

Oil Shale Process Model (OSP) User's Manual

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Oil Shale Process Model

(OSP)

User's Manual

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PREFACE

The Oil Shale Process (OSP) model has proven to be a useful tool for the analysis of the steady-state operation of Lawrence Livermore National Laboratory's Hot-Recycled-Solids 4 tonne-per-day Pilot Retort (4TU-Pilot). This manual is being developed to serve as a guide to users of the OSP model.

The OSP code is being developed for generalized chemical process simulation of the HRS oil shale retort. Several of the common unit operations encountered in industrial chemical process design are included in the OSP code, including packed and fluidized bed reactors, splitting and mixing operations, and a dilute flow lift-pipe. A set of chemical species and reactions related to oil shale processing are available for incorporation into a given simulation.

This manual will guide an engineer/programmer through the setup, execution and analysis of an OSP simulation. Two other manuals complete the documentation for the OSP code, the "Oil Shale Process Model (OSP) Theory Manual" and the "Oil Shale Process Model (OSP) Code Development Manual." These manuals should be referenced when additional information on underlying theories or program structure is required.

INTRODUCTION

The computer code OSP has been developed to allow a generalized-steady-state-numerical simulation of the Hot-Recycled-Solids (HRS) Oil Shale Process to be constructed. The HRS process is being developed at Lawrence Livermore National Laboratory (LLNL) for the above ground retorting of oil shale. The OSP code helps research staff to critically analyze operation of LLNL's 4TU-Pilot. It can also be used to test the consistency of the laboratory data as well as the pilot scale results.

The OSP code uses information contained in a user supplied input file to select the order, number, and type of computational unit operations used in a simulation. The chemical species and the number and type of chemical reactions occurring in a unit operation are also specified in the input file as are initial estimates for processing conditions, stream flow rates, and chemical compositions.

This manual describes the details of constructing an input file for OSP, steps needed to run the code, rerun and post run options. First, the computational modules available in OSP are outlined. This is followed by a description of the nature of the streams used to connect the process modules. A summary description of the I/O files used by OSP follows. The suite of reactions from which the user can select is next outlined and then a description of execution options for the code are given in some detail. The final section briefly describes a companion post-processing code, TAB, which can be used to obtain additional information about simulation runs.

A great deal of information is contained in the five appendices. The first appendix gives detailed information about all the input options. The remaining four describe four example runs. Within the discussion of these examples a considerable amount of information is available about actual operation of the code. It is strongly recommended that the user review these examples before generating his own input file.

UNIT OPERATION MODULES

In this section, the computational modules presently in the OSP code are briefly described. Some references to input parameters are made, but for a complete list see Appendix A. Before describing each module a discussion of common features of the reactor modules is presented.

There are eight modules in which chemical reactions or changes in phase can be performed. Two of these are based on simple material and energy balance considerations. These are the PHASE_CHANGE and STOICH.REACT modules which allow simple phase changes to be performed in the case of the PHASE_CHANGE module, and allow reactions to be carried out based on input of the extent of reaction in the case of the STOICH.REACT module.

The other six modules which allow reactions to occur are based on assumed kinetic models. In addition, they make assumptions as to the nature of the flow and as a consequence have models to compute energy transport between solids and gases. This group of 6 modules are the primary computational modules of OSP and represent different types of reactors. These reactor modules make use of two underlying computational models, the plug-flow model and the well-mixed model. These underlying models define the basic flow geometry. In the plug-flow model it is assumed that all materials are moving co-currently in a single direction, however the velocities of various components may be different. In the well-mixed model it is assumed the system is well-mixed and there is therefore no spatial resolution. The CO_CURRENT, LIFT_PIPE and PACKED_BED modules use the plug-flow model while the CNTR_CURRENT, CSTR and FLUID_BED modules make use of the well-mixed model.

In reactor modules using the well-mixed model there is an ability to define the way in which average properties of the gases, solids and liquids are determined. These average values are used to compute transport properties and reaction rates. The most robust assumption is that these average properties are equal to the exiting properties. This is the classical assumption for a cstr (continuously-stirred-tank reactor) and in general allows a satisfactory solution for output streams to be found regardless of inlet stream composition. It may be that some other weighting involving inlet and outlet streams is desired and input parameters (WEIGHT_GAS_IN WEIGHT_SOL_IN, and WEIGHT_LIQ_IN,) are provided for this purpose.

The user is cautioned to clearly consider the consequences of using anything but the default values for weighting factors. For instance, consider the case in which oxygen enters a reactor along with a solid stream containing carbon. Assume that the system is hot so combustion reactions are fast and there is more oxygen than needed to completely combust the carbon. With the classical cstr assumption a module using the well-mixed model will probably successfully find a solution in which the carbon content of the exiting solid is very near zero. Even though very small, this carbon concentration yields a computed combustion rate necessary to consume essentially all the incoming carbon. On the other hand, assume that a 0.5 weighing factor was used for the solid averages. This means that the carbon content used in computing reaction rate would be the average of the inlet and outlet carbon content. If negative concentrations are not allowed it is clear that no solution could be found for this case since computed reaction rates using carbon content equal to half of the injected content would lead to carbon consumption rates far greater than the rate of carbon entering the system. In general nothing but zero weighing of injected streams should be used for phases containing a limiting reactant

Each of the reactor modules have common options associated with selection of desired species and reactions, and the definition of basic reactor geometry. For all reactors the size is defined by a DIAMETER and a HEIGHT. Reactor volume is computed simply using a formula for a cylinder. The selection of species and reactions is controlled by

the setting of a series of flags. Details of setting these flags is described in the "Selection of Species and Reactions" section.

Transport between gases and solids is controlled in each reactor module through the use of two flags, IBED and IDILUTE. The IBED parameter determines the types of correlations used in computing mass and heat transfer coefficients between particles and gas. Two sets of correlations are available, one more appropriate for dilute phase system which relies on single particle correlations, and the other more appropriate for dense phase systems in which packed bed correlations are used. The IDILUTE parameter determines the solid particle size to use in the transport correlations. Again two options are available, one in which the particle size of the solid stream under consideration is used directly, and another in which an area (diameter squared) weighted particle size is used. In the later case the module uses particle sizes from all input streams to determine the single diameter to use in computing transport coefficients for all particles regardless of their size. In each of the reactor modules these parameters are defaulted to values most appropriate to the most common use of the module. In certain cases like the LIFT_PIPE and the PACKED_BED modules these choices are obvious, but in others they are not. The user is cautioned to check the default values and reset them if appropriate.

Each of the reactor modules requires one gas inlet and outlet stream to be defined. A single liquid inlet and outlet stream can be optionally specified. A set of up to 10 pairs of solid inlet/outlet streams may be defined.

For the most part, the reactor modules are primarily concerned with gas and solid phases. The current implementations include liquids in only approximate fashions. For example, the liquid stream in a reactor module is assumed to have the same temperature as the gas phase, also when velocities are required the liquid phase is assumed to have the same velocity as the gas. One reactor module, the STOICH.REACT module, is the exception to the equal temperature assumption. In this reactor module computations based on input stoichiometric factors are performed and as a consequence details of solid, liquid and gas interactions are not required and the liquid phase is allowed to have a temperature different than the gas phase.

In modeling an actual physical unit with these reactor modules it is often appropriate to use several modules hooked together to perform the require computations. This is particularly appropriate if one is modeling a truly counter-current reactor. In this case using a number of CNTR_CURRENT modules in series will give an approximation of spatial variations which may be present in such a system

ATTRITION Module

The ATTRITION module is used to simulate the changes in particle sizes that occur in the processing of oil shale. Because the mechanism responsible for the attrition can differ at different locations in the process a number of different types of attrition are

available to the user. TYPE=1 attrition assumes that the composition of a solid particle that is to undergo attrition is uniform spatially. The mass fraction of solid that attrits in this module is an input parameter. The chemical composition of the original, parent solid particle and the daughter materials generated in the attrition process are the same. A solid stream with a single particle size can be broken up into as many as 10 daughter streams each with its own diameter. The user supplies values which sets the fraction of the parent stream which is transformed into each daughter stream and the size of the particles in each new stream. TYPE=4 attrition is essentially the same, except only two output streams are allowed. The diameter of the first stream is derived from that of the input stream by assuming loss of the required fraction of mass. The second stream has a diameter set by user input. TYPE=5 attrition is also essentially the same as TYPE=1, except that the size of the newly created particles are not given explicitly, but are instead specified as a fraction of the original particle size.

In TYPE=2 and 3 attrition, it is assumed that the parent stream gives rise to only two daughter streams. The composition of the parent particle and the daughter streams are in general different. This type of attrition is typically used to simulate the attrition of a particle that has an ash layer at its surface. The ash layer differs from the material in the interior of the particle because it has been depleted of carbon (char). The chemical composition and density of the char are obtained from stream variable information of the parent particle. In TYPE=2 attrition, it is assumed that a specified mass fraction of this exterior layer of ash is attrited. In TYPE=3 attrition, it is assumed that the layer thickness of the ash is maintained equal to or less than a specified value. If a particle enters the module with an ash layer greater than the specified thickness the particle attrits to a new particle size which has an ash layer equal to the specified value. In both cases the diameter of the attrited ash particles is a user defined parameter.

Finally, a TYPE=6 attrition is available which is essentially the same as TYPE=2 attrition except that the amount of material to be attrited is not specified as a fraction of the ash layer weight, but rather as the fraction of the total weight. Material needed to generate the specified attrition is first taken from the computed ash layer. If more material is needed, material is taken from the char enriched core.

BALANCE Module

The BALANCE module performs overall balances on the selected streams. Overall atom and energy balances are performed as well as kerogen-oil-coke balances useful in analyzing overall oil generation performance. This module can accept up 40 stream connections (sum of both input and output).

CNTR_CURRENT Module

The CNTR_CURRENT module is a reactor module tuned to allow a dilute solid phase counter-current flow reactor to be modeled. This module assumes that the process to be

modeled is basically one in which solids and gases/liquids move in a counter-current fashion relative to each other. No spatial resolution is assumed and the well-mixed model is used to perform the required computations. The default assumption for transport correlations in this module is that single particle correlations using actual particle sizes are appropriate.

The well-mixed model requires effective densities of each component to be specified for reaction rate computations, as well as relative solid-gas velocities for use in transport correlations. Effective densities of solids in the reactor are determined by the user specified velocities for each solid stream, the HEIGHT of the unit, and input solid flow rates. The effective gas density in the reactor is computed from the averaged properties as defined by the gas weighting factor (for default outlet conditions are used). This module assumes the solid density in the reactor is small and it assumes the gas volume in the reactor is equal to the reactor volume. This means this module will not perform well for dense phase systems. Solid-gas velocities used in transport correlations are computed by adding the solid velocities, specified by the user, to the average gas velocity. The average gas velocity is computed using average gas properties and assuming the gas flow along the HEIGHT of the unit.

Since this reactor module was conceived to primarily look at dilute phase systems an additional heat transfer mechanism can be invoked if desired. This mechanism is meant to make some allowance for radiative heat transport from the solid material. The basic assumption is that the particles radiate to a wall and the wall then transfers heat to the gas phase. The model adjusts the wall temperature until a balance between solid to wall and wall to gas is obtained. The net effect is to enhance the heat transfer between solid and gas.

CO_CURRENT Module

The CO_CURRENT module allows a dilute phase co-current plug-flow type reactor to be modeled. The PACKED_BED module should be used for dense phase systems. The gas and all solid streams may have separate velocities. This module uses the internal plug-flow module to perform the actual calculations consequently spatial changes are resolved in the course of the computations and spatially resolved results can optionally be written to a special output file.

The plug-flow model uses velocities set by the user for each solid stream and it is assumed that these do not vary as they move along the HEIGHT of the reactor. Superficial gas velocities are computed as needed and use local values of temperature and total gas flow rate. Gas-solid velocities are computed from the difference between the superficial gas velocity and the solid velocities. The default assumption for transport correlations in this module is that single particle correlations using actual particle sizes are appropriate.

Since this reactor module was conceived to primarily look at dilute phase systems an additional heat transfer mechanism, similar to that described above in the CNTR_CURRENT module, can be invoked if desired. This mechanism is meant to make some allowance for radiative heat transport from the solid material. The basic assumption is that the particles radiate to the wall and the wall then transfers heat to the gas phase. The model adjusts the wall temperature until a balance between solid to wall and wall to gas is obtained. A further simplification is used in that the equilibrium is invoked at each slice across the reactor, no provision is made for radiative transport in the axial direction. The net effect is to enhance local heat transfer between solid and gas.

This module also allows an additional heat source/sink to be defined between reactor wall and gas phase. This is implemented as a heat transfer term which uses a wall to gas heat transfer coefficient and a user defined wall temperature. The user can selected a fixed value for the heat transfer coefficient or instruct the module to compute an appropriate heat transfer coefficient based on correlation for gas flow inside a circular conduit.

CSTR Module

The CSTR module simulates a cstr reactor. The default parameters are tuned to represent a simple fluidized bed system with no bubble phase. No spatial resolution is assumed and the well-mixed model is used to perform the required computations. The default assumption for transport correlations in this module is that single particle correlations using a single average particle size are appropriate.

The well-mixed model requires effective densities of each component to be specified as well as relative solid-gas velocities for use in transport correlations. Effective densities of solids in the reactor are determined by the user specified void volume fraction in the reactor, BEDP. The distribution of solid streams within the reactor are determined, by default, from the ratio of input solid flow rates. Alternatively the user can choose to specify the relative fractions of each input stream within the reactor. Provisions are provided to allow the user to group input streams in specifying this distribution. The effective gas density in the reactor is computed from the averaged properties as defined by the gas weighting factor (for default outlet conditions are used) and the bed porosity. A single solid-gas velocity is used in transport correlations for all particles. This velocity is the superficial gas velocity through the reactor assuming the direction of gas flow is along the reactor's HEIGHT. The properties and flow rate of the gas is taken from available estimates of the outlet gas properties.

ERROR Module

The ERROR module allows error criteria to be set on stream variables. This provides a means to insure convergence of stream properties other than temperatures. This module can accept up 40 stream connections.

FLUID_BED Module

The FLUID_BED module allows a two phase fluidized bed reactor to be modeled. A bubble phase and an emulsion phase are assumed to be present in the reactor. A fluidized bed reactor is one in which a fluid is passed up through particulate solid at a velocity which is great enough to cause the solid to become levitated. Bubbles form at the bottom of the bed and pass up through the denser emulsion phase. The FLUID_BED module divides the reactor into as many as 5 vertical sections. The number of sections is set by the user and is meant to determine how many bubbles are in the bed at any one time. The emulsion is assumed to be well mixed throughout the emulsion region of the reactor and the bubbles are assumed to move from the bottom of the reactor through the vertical sections to the top of the reactor. At the top of the reactor the gases from the bubble and emulsion phases are mixed. A modified version of the well-mixed model is used to perform the actual calculations.

The split between the flow of gas in the emulsion phase and the bubble phase is determined from an internal correlation, as are the bubble size and the exchange rate between gases in the bubble and emulsion phase. The total amount of the gas in the bubble phase is computed from the size and number of the bubbles. The gas volume in the emulsion phase is set by the user supplied bed porosity parameter, BEDP, the reactor volume and the volume of the bubble phase. BEDP is the void volume fraction of the emulsion phase. Effective densities of solids in the emulsion phase, and therefore the reactor, are determined by the user specified void volume fraction. The distribution of solid streams within the emulsion are determined, by default, from the ratio of input solid flow rates. Alternatively the user can choose to specify the relative fractions of each input stream within the emulsion. Provisions are provided to allow the user to group input streams in specifying this distribution.

A single solid-gas velocity is used in transport correlations for all particles. This velocity is the superficial gas velocity through the reactor assuming the direction of gas flow is along the reactor's HEIGHT. The properties and flow rate of the gas is taken from available estimates of the outlet gas properties.

LIFT_PIPE Module

The LIFT_PIPE module allows a dilute phase lift-pipe to be modeled. The lift-pipe is assumed to behave like a plug-flow reactor, with solid-gas slip. This module uses the

internal plug-flow model to perform the actual calculations consequently spatial changes are resolved in the course of the computations and spatially resolved results can optionally be written to a special output file.

The velocities of each of the solid particle size classes and the gas are either supplied in the input file as a slip velocity relative to the gas velocity or they are determined using a momentum balance procedure. When a momentum balance is performed, the effects of solid-solid impact and solid wall friction are included in the calculation. The velocities are calculated using the gas and solid properties at the entrance of the lift-pipe. At the end of the calculation, the calculation of solid velocities is repeated using the properties at the final computed exit conditions, for comparison.

The default assumption for transport correlations in this module is that single particle correlations using actual particle sizes are appropriate. A radiant transport mechanism and a wall-to-gas heat transfer term exactly like that described for the CO_CURRENT module may also be selected if desired.

MERGE_STRMS Module

The MERGE_STRMS module combines multiple input streams into a smaller number of output streams. All output streams are in thermal equilibrium (i.e. same temperature). The outlet temperature is determine by adiabatic mixing of all input streams in the absence of any reactions. Only one gas and one liquid stream can leave the module but multiple exiting solid streams can be defined by specifying group membership. A maximum of 10 solid groups can be defined. This module can accept up 40 stream connections (sum of both input and output).

PACKED_BED Module

The PACKED_BED module allows a dense phase co-current plug-flow type reactor to be modeled. The CO_CURRENT, or LIFT_PIPE modules should be used for dilute phase systems. This module uses the internal plug-flow model to perform the actual calculations consequently spatial changes are resolved in the course of the computations.

The plug-flow model uses velocities established by the user selected bed porosity, BEDP, and the inlet solid flow rate. All solids move at the same rate and it is assumed do not vary as the solids move along the HEIGHT of the reactor. Superficial gas velocities are computed as needed and use local values of temperature and total gas flow rate. Gas-solid velocities are computed from the difference between the superficial gas velocity and the solid velocity. The default assumption for transport correlations in this module is that packed bed correlations using a single particle size are appropriate.

PASS_THRU Module

The PASS_THRU module passes input streams straight through to output streams. This module is useful in making name changes and in isolating recycle loops. This module can accept up to 40 stream connections (sum of both input and output).

PHASE_CHANGE Module

The PHASE_CHANGE module allows the thermal effects of phase changes between gases and liquids to be determined. Simple material balance algorithms are used in this module. No phase equilibrium considerations are included. Two types of phase change are handled: condensation, TYPE='C', and evaporation, TYPE='E'.

When executed in the condensation mode, the module condenses selected components from an input gas stream and generates a separate liquid stream for each species condensed. Only those gas species having a corresponding liquid species may be condensed. The user must provide names for each of the condensed liquid streams. There is a single temperature for the exiting gas and liquid streams. This temperature is either specified by user input or if user input is absent the temperature of the input gas stream is used. Heat effects involved in the condensation (or evaporation) can be determined by examining the energy balance portion of the ASCII output.

In the condensation mode, this module can also be used to heat/cool a gas stream. When used in this fashion an input and output gas stream are specified and the desired temperature set. No species are specified for condensation and no liquid streams need be declared.

In the evaporation mode, the module allows selected species in an input liquid stream to be evaporated into a gas stream. All liquid species can be evaporated. In this mode an input liquid stream and an output liquid and gas stream must be specified. An input gas stream is optional.

PROP_TAB Module

The PROP_TAB module is a service module that prints out a table of all species properties over a selected range of temperatures. It can optionally output mixture properties for solid, gas and liquid streams. Up to 40 streams can be specified. This module plays no active part in a simulation. Unlike most other modules the computations done by this module are all done during the initialization phase. Results are printed in the ASCII output file at the same time other modules are only printing out input variables. This module performs no calculations during the calculation phase of OSP's execution.

RELAX Module

The RELAX module allows solid stream updating which blends old and new values of solid stream parameters. The module gives the user some control over which properties are relaxed. This relaxation to newly computed values is sometimes necessary to allow the steady-state condition of a recycle loop to be reached without going into oscillations. A total of 10 in/out solid stream pairs can be defined.

SPLIT_STRMS Module

The SPLIT_STRMS module allows single streams to be split into two output streams. The splitting can be done on a fractional bases or an absolute flow rate level can be specified for one outlet stream with the other carrying the remainder of the flow. It is also possible to use this module to multiply a stream flow by any real value. Only one input gas and one liquid stream are allowed. Up to 10 solid input streams can be defined. For cases in which a desired solid flow rate has been selected the flow rate is applied to the sum of all the solid streams. The required solid is take in equal fraction from each input stream.

STOICH Module

The STOICH module determines the stoichiometry of a given reaction. Also, the heat of reaction over a selected temperature range can be computed and listed to the ASCII output file. The user can optionally use the module to reset stoichiometric coefficients of a reaction. Unlike most other modules the computations done by this module are all done during the initialization phase. Results are printed in the ASCII output file at the same time other modules are only printing out input variables. This module performs no calculations during the calculation phase of OSP's execution.

This module uses the stream information in a special way. Specification of stream composition and flow are used to set known stoichiometric coefficients of the reaction. As a consequence negative mole fractions or weight fractions are meaningful and are used to designate reactants. The input composition multiplied by the streams flow rate are interpreted as the known stoichiometric coefficients. A single stream is used to specify all components of a given type. No more than three streams are needed a solid, a gas and a liquid stream. The specification is completed by defining the reactants whose coefficients are to be computed and which atomic balances are to be employed. The user should also select a "base" component. Results will be normalized so that this "base" component has a coefficient of one. It is the user's responsibility to pose a well defined problem. The module does some consistency checking and will report an error if it can determine the set of equations it needs to solve is under or over defined.

STOICH.REACT Module

The STOICH.REACT module allows the extent of specified reactions to be set by input parameters. The specified reactions are performed and appropriate energy and material balance constraints are imposed. The extent of reaction is specified based on input reactant levels and is based on the limiting reactant for a specified reaction. One input gas and one liquid stream are considered, but multiple input solid streams are handled. Since stoichiometry is done relative in inlet amounts, two step processes require the use of multiple modules. Also it is possible to specify input parameters which would require more than the available amount of a reactant to be consumed. This can occur when a reactant is consumed in more than one reaction. If this occurs an error message is given and calculations are terminated. The user can then take action, such as splitting the module into two modules, to get the desired computations performed with no ambiguity or error.

Several options are available for specifying the temperature of the material leaving the reactor. First an adiabatic option is available in which all exit temperatures are assumed equal and the value of this temperature is based on an overall energy balance . A closely related option is available where adiabatic operation is assumed with the exception that an energy flux into or out of the system can be specified independent of the mass flow streams. Finally, an option is available which allows the temperatures of the streams exiting the reactor to be fixed. In this case the required heat gain/loss to satisfy an energy balance is computed as part of the calculation.

PROCESS STEAMS

In the OSP code, unit operation modules are connected with process streams. Three types of process streams are used; gas streams, solid streams and liquid streams. The units for the flow rate used for gas streams are mol/s and the units for the flow rate for solid and liquid streams are kg/s. The temperature (in K) and the composition of a stream are also included as part of the stream characterization. The units of composition of gas streams are mole fractions and for solid and liquid streams they are mass fractions. The particle size (in meters) is also part of a solid stream characterization. If a distribution of solid size classes is used, then the distribution can be discretized into several separate streams each with appropriate particle size and flow rate.

All streams are designated by a name which is up to eight characters long and is not case sensitive. In the current OSP code there are provisions for 100 gas streams, 400 solid streams and 10 liquid streams. It is a relatively simple task to increase these limits. Refer to the "Oil Shale Process (OSP) Code Development Manual" for procedures to increase these values.

In general properties of streams are the result of computations, however certain process stream variables need to be initialized by the user. Each input stream to the overall

process needs to be set and this is done using the appropriate \$INIT group. Streams may also need to be initialized to act as initial guesses for certain computational modules (e.g. the CSTR module) or certain recycle streams. Good initial guesses can make solutions easier to obtain, but this needs to be weighed against the complexity of the input file. In a complex process if too many initial guess are made explicitly in the input file then a change in operating conditions may require a change to many of the initialized streams. It is recommended, therefore, that initial guesses for streams be kept to a minimum. Most of the modules which need initial guesses for output streams have algorithms for obtaining them from internal information. This generally involves using an input stream as an initial guess or using some other stream not necessarily connected to the module for this purpose.

All process streams have all process variables defaulted to zero. This default value is used by some modules to signal if special attention needs to be given for initial guesses as outlined above. Provisions are also provided to initialize all streams to values found in a previous computation. These values either overwrite stream initializations given in the ASCII input file or are overwritten by initializations declared in the input file.

There are three types of \$INIT specifications: \$INITGAS for gas streams, \$INITLIQ for liquid streams and \$INITSOLID for solid streams. Care should be used in defining the specifications for the streams so that all parameters are specified. For instance if a particular calculation is desired for a gas stream but the results are not believed to be influenced by pressure and the user has no particular pressure level in mind it is prudent to select an arbitrary level since internal calculations may make use of the pressure even though in the case of interest its value is arbitrary. Similarly for solid streams particle size should in general always be specified. A list of stream variable options is available in Appendix A.

OSP FILES

OSP makes use of four primary I/O files during its execution. These files include the input file which is assumed to have the suffix ".inp", the ASCII output file which is given a ".dat" suffix by OSP, a stream file which is given a ".strm" suffix, and the binary-common-space-storage file which is given a ".mod" suffix. The user needs to be aware of the contents and use of all but the ".mod" file. The ".mod" file is used only by OSP itself and is not meaningful once a run has been completed.

The input file (the ".inp" file) is an ASCII file in which the user places all the information necessary to setup a simulation. All input variables in the file must belong to an input group. An input group is declared by specifying a '\$NAME', where NAME is one of the following:

\$GLOBAL - A limited number of control parameters.

\$PROPERTIES - Species and reaction related parameters.

\$FLAGGAS - Set up gas use flags to be used in module definitions.

\$FLAGSOLID - Set up solid use flags to be used in module definitions.

\$FLAGLIQ - Set up liquid use flags to be used in module definitions.

\$FLAGREAC - Set up reaction use flags to be used in module definitions.

\$MODULE - Module definition group.

\$INITGAS - Group used to initialize values of a gas stream.

\$INITLIQ - Group used to initialize values of a liquid stream.

\$INITSOLID - Group used to initialize values of a solid stream.

Detailed information on the constructing an input file and a complete listing of all input parameters is available in Appendix A.

OSP always generates two output files which contain the results of the simulation. These are the ".strm" and the ".dat" files. The ".strm" file is a binary file containing information about the state of all process streams. This file not only contains the state of these streams at the end of computations but also contains a record of intermediate states during execution. Depending on the setting of control variables a complete snapshot of all stream variables are written to this file after execution of calculations associated with each defined process module, or alternatively the results are written only at the end of each computational loop. A computational loop is defined as the execution of all defined modules one time. In recycle systems multiple loops are required to reach a fully converged solution . This stream file has two primary uses. It can be used to obtain stream information for use in restarting a simulation or initializing stream variables for a new simulation. The new simulation may just be a run where additional information about the primary run is obtained using selected modules to present alternative information (Appendix C gives an example of this use). The ".strm" file is also used by the TAB code to generate additional output not available in the ASCII output file.

The ASCII output file, the ".dat" file, contains the results of the run as well as a complete listing of all user selectable parameters. The contents of the file are mostly self explanatory and will not be dealt with directly here. A fairly complete discussion of the contents of this file is available in the descriptions of the example problems given in Appendices B-E.

Two of the modules, LIFT_PIPE and CO_CURRENT, are also able to write out additional data files. These files contain selected spatially resolved data. Two formats

for this data can be chosen. The first is simple an ASCII format option which produces a file directly readable by the user. A second option allows a particular type of binary file to be generated which can be used as input to special display software. This later format is only useful if the computer system in use has the "hmp" software. This software was developed locally within the LLNL energy projects and is not generally available at other locations.

SELECTION OF SPECIES AND REACTIONS

In the current OSP version, there are 28 gas species, 8 liquid species and 34 solid species. In addition, reaction modules can select from a series of 25 reactions involving these species which have predefined kinetics and stoichiometry and an additional 4 reactions with no predefined stoichiometry.

A complete list of available species are listed in Appendix A. Most of these compounds are familiar, but a few require some further description. There are three kerogens in the list (Kerogen-1, Kerogen-2 & Kerogen-3). Presently, only Kerogen-1 is fully integrated into the reaction scheme. Kerogen-2 and Kerogen-3 were included to accommodate a future implementation of a more elaborate kerogen pyrolysis reaction. The other solid organic carbon containing species are char and coke. For the most part we define char as the residue left from primary pyrolysis of kerogen and coke as the solid residue from secondary pyrolysis of oils. To accommodate future kinetic models for char combustion char can be represented in one of two ways. The first method represents char using 5 solid species, one for each of its atomic components (carbon, hydrogen, oxygen, nitrogen and sulfur). This has the potential to allow different rates of consumption of char by combustion based on its current composition. The second method is more computationally economical and represents char as a single solid species with a fixed composition. This composite char species should be used unless special circumstances or needs require the use of the more elaborate char species model.

The solid species list includes several other components requiring special comment. Two water species are included, one representing physically bound water (Moisture) and the other chemically bound water (Bound-Water). A number of oil species are included which are meant to represent oil adsorbed on the solid. Finally four generic solid species labeled by default SOLID-A through SOLID-D have been included. These species are place holders and allow the user to define solid species not present in the default list. Provisions are available in the \$PROPERTIES group to rename these, or any other solid, as required by the user needs.

In the gas species list there are two purely artificial species, C5 and H12 which have been included for possible use in closing pyrolysis material balances. They are currently not used but could be used to represent production of hydrocarbon gases with a specified hydrogen/carbon ratio. Finally, five oils have been included. These are present in both the gas species list and the liquids list which allows for their presence in

the system in either form. Currently, only three of the oils (Oil-1, Oil-2 and Oil-3) are actively used. As in the solid list four generic gas species have been included to provide the user with the ability to define new gas species.

Only eight species have been included in the liquid list. Five oils, water and two generic species. This list is small because OSP's primary focus is on gas solid interactions and its ability to handle liquid species is limited. As with solids and gas species liquid species' names can be redefined by the user.

The user should understand that renaming a species does not provide the necessary compositional and thermodynamic parameters necessary for its effective use in OSP. When a name is changed the user needs to review all pertinent data (see the appropriate section in the \$PROPERTIES area in Appendix A) and define or redefine those parameters which will be needed in the calculations. Also the user should carefully weight the action of renaming any but the generic species. Many of these species are referenced in kinetic expressions and the reference is not by name but by a sequence number.

Those species included in at least one internally defined reaction (see Appendix A) include:

Solid Species - Kerogen-1, Kerogen-2, Kerogen-3, Char-C, Char-H, Char-O, Char-N, Char-S, CaCO₃, CaO, MgCO₃, MgO, SiO₂, CaSiO₃, FeS₂, CaSO₄, Oil-1, Oil-2, Oil-3, Char and Coke.
Gas Species - N₂, O₂, H₂, CO, CO₂, H₂O, H₂S, SO₂, NH₃, NO₂, CH₄, C₂H₄, C₃H₆, Oil-1, Oil-2 and Oil-3.
Liquid Species - Oil-1, Oil-2 and Oil-3.

In many of the simpler modules the user is not required to make any selection of species or reactions since they always work with the full suite of species. On the other hand, the six reactor modules CNTR_CURRENT, CO_CURRENT, CSTR, FLUID_BED, LIFT_PIPE and PACKED_BED require the user to make a selection of species and reactions to consider. The reason for this is two fold. The primary reason is that these modules tend to be computationally intensive and the computer time goes up as more species are considered, therefore to improve the efficiency of the solution only those species considered important in a unit should be considered. The second reason is to give additional control over processes occurring in the module. Sometimes it may be desirable to guarantee that a particular reaction does not occur that normally would, reaction selection gives the user this option.

The primary way of selecting species in the reaction modules is by declaring it in the module input. The declaration is done with a code word and species or reaction name. The details are given in Appendix A under "Block A Parameters." Each reaction module requires a single set of declarations to be defined for gas species and liquid species. For solids, on the other hand, a declaration is required for each solid input stream. This allows the module to follow different solid species in different solid streams. Often,

however, the same species are to be followed in each solid stream. For this case a parameter, SOLSAME, is provided which notifies the module that species declarations all solid streams not yet explicitly set are to be set in the same manner as the last set defined.

When a species is not declared for a reaction module the quantity of that species is explicitly set to zero in the output streams from that module. Consequently, if it is desired to keep track of any species, even if it has a small quantity and does not partake in any reactions in a given module, that species should be declared.

One consideration in selecting reactions for reactor modules is that all species participating in a selected reaction are included in the active species list. Available reactions and species they involve are listed in the Appendix A under "Stoichiometric defaults ...". OSP does a consistency check to be sure that all necessary species have been selected. However, it gives the user the option to proceed even if there is an inconsistency. Care must be taken in proceeding with a system where species are missing since effective heats of reaction are computed on the basis of active species. Still, in some circumstances the knowledgeable user may choose to perform a calculation even with some reaction/species inconsistency.

OSP provides a short cut means of specifying species and reaction flags, especially useful in cases where the same groups of species and/or reactions tend to be required for several modules. This is through the use of the \$FLAG specifications. There are four different flag groups, \$FLAGGAS, \$FLAGLIQ, \$FLAGSOLID and \$FLAGREAC for specifying gases, liquids, solids and reactions respectively. Each \$FLAG section includes a name and a list of desired species or reactions as appropriate. As many as 40 different \$FLAG areas can be defined. Flags are set in the various reaction modules by setting the GAS_FLAG, LIQ_FLAG, SOL_FLAG, REACT_FLAG to the appropriate \$FLAG name. In the \$FLAGSOLID area only one set of solid species flags can be set. That is, multiple stream flags are not supported.

PROPERTIES

The \$PROPERTIES area of the input file is used to set various species and system properties. For all parameters default values are set by OSP. The values of the default values can be determined by examining Appendix A. However, any execution of the OSP code will result in a listing of these defaults.

Among the required parameters are species properties used by the computational modules. Default values for specifying various species properties are listed in Appendix A under the heading "Data statements from the props.f file". The user can modify certain of these default values by setting the appropriate variables. Those species properties which can be modified by entries in the input file are:

Gas Species -	name, heat capacity, heat of formation, atomic composition, molecular volume, and viscosity.
Liquid Species -	name, heat capacity, heat of formation, and atomic composition.
Solid Species -	name, heat capacity, heat of formation, atomic composition, and density.

A gas/solid transport parameter used by the reaction modules can also be set in the \$PROPERTIES section. This is the particle sphericity used in computing gas/solid mass, heat and momentum transport.

The remainder of the parameters selectable in the \$PROPERTIES section are kinetic parameters for the available OSP reactions. For all reactions the stoichiometric parameters can be redefined from the internal default values by including the appropriate entries. The stoichiometric parameters are G_STOICH, L_STOICH and S_STOICH. These are defined in Appendix A. The STOICH module can be used either in the same OSP run or in a separate run to assist in the setting of alternate stoichiometric coefficients. An example of using the STOICH module is provided in Appendix D.

In setting \$PROPERTIES parameters tied to a particular species or reaction index numbers, not species or reaction names are used. The user can obtain the proper index number by consulting a previous run or using the lists provided in Appendix A.

Available reaction parameters and a brief description of other selectable parameters is provided in the next section. For a more thorough description of the reactions and kinetic expressions please see the companion report "Oil Shale Process (OSP) Theory Manual."

REACTIONS

Currently OSP contains a set of 29 reactions which can be selected in each of the reactor modules. The first 25 of these have predefined reaction stoichiometry. The last four are generic reactions for which the user can define his own stoichiometry without impacting any of the default settings. In addition the first 25 defined reactions have kinetic expressions available.

The first three defined reactions are used to describe combustion of three types of kerogen. These reactions are included to remove any small amounts of kerogen which may find their way into an oxidizing atmosphere. The kerogen is assumed to combust at a rate equal to its pyrolysis rate. OSP automatically sets the products of combustion to the appropriate quantities of CO₂, H₂O, SO₂, and NO₂ based on the composition of the kerogen. No kinetic parameters are directly selectable in the input file. However,

kerogen decomposition parameters describe below are used for all three reactions to set their basic rates.

The next five reactions are used to describe the burning of the char species defined as individual atomic components one each for carbon, hydrogen, oxygen, sulfur and nitrogen. All are tied to a single kinetic formulation based on a shrinking core model. Selectable parameters include the initial char density for use in the geometry parameters of the shrinking core model, a frequency factor and an activation temperature for use in the basic kinetic rate, and a kerogen density and a multiplicative factor used in computing effective oxygen diffusivity into the combusting particles. The initial char density and the kerogen content are set for a stream by setting the PROP(1) and PROP(2) stream properties respectively.

Reactions 9 and 10 specify direct magnesium carbonate and calcium carbonate (calcite) decomposition respectively. A set of frequency factors and activation temperatures can be set for these reactions.

Reactions 11 and 12 describe the pyrolysis of Kerogen-1. Reaction 11 assumes products will include oils in liquid form while reaction 12 is identical except default stoichiometric factors assume that oils are produced as gases. The solid carbonaceous residue is assumed to be the composite char specie with an assumed default composition. A frequency factor and an activation temperature can be specified. These are the same factors mentioned above which are used in the description of kerogen combustion.

Reactions 13-18 are used in the description of the coking of oils 1-3 on solid surfaces. The first three of these reactions describe adsorption/desorption of oils from the gas phase onto and from the solid particle surfaces. The last three describe coking of oils on the solid surfaces to produce coke and gaseous products. Selectable parameters include the effective internal surface area of the solid particles, the density of coking sites on the surface, an definition of the average length for oil diffusion into out of the solid particles, the relative coking rate on clean and coked surfaces, and a set of frequency factors and activation temperatures defining adsorption isotherms and coking kinetics.

Reaction 19 describes the combustion of coke in the solid particles. A frequency factor and an activation temperature can be specified as well as an average length parameter defining the relative distance for oxygen diffusion inside the particles.

Reactions 20-22 allow for the vaporization of liquid oils 1-3. These rates are not based on a physical model. They are included only to allow heat effects for oil vaporization to correctly integrated into a reactor module. The assumption is that the oils will evaporate rapidly and essentially to completion. A set of three scale factors can be input to modify the rate of vaporization. Values should be used that provide for rapid enough evaporation to vaporize all the liquid oil but not so fast as to cause undue difficulties in the computations of a given reactor module. Defaults values should be tried first and then adjusted as needed.

Reactions 23-24 describes the combustion of composite char and the combustion of FeS₂. An approximate shrinking core model similar to that used for the individual char species combustion is used. The size of the combustible core is computed individually for each reaction based on remaining char and FeS₂, but the oxygen flux used is that for both char and FeS₂ combustion. This formulation is an exact representation of a shrinking core combustion when only one reaction is active. When both reactions are active the true situation is quite complicated, as it is if coke or kerogen combustion is also occurring. In these cases the formulation can be counted on to behave in a smooth fashion and give reasonable combustion rates. The same selectable parameters as employed in the species char combustion reactions are used for the char combustion kinetic model. A similar set for the FeS₂ are also available. The parameters include the initial char or FeS₂ density for use in the geometry parameters of the shrinking core model, a frequency factor and an activation temperature for use in the basic kinetic rate, and a kerogen density and a multiplicative factor used in computing effective oxygen diffusivity into the combusting particles. The initial char density is set for a given solid using stream PROP(1), the original kerogen content is set using PROP(2) and initial FeS₂ density is set using PROP(3).

Reaction 25 describes a kinetic model for carbonate decomposition via a reaction with SiO₂ to form CaSiO₃. A set of frequency factors and activation temperatures can be set for this reaction.

GENERAL COMPUTATIONAL SCHEME

Computations within each module are performed independent of other modules. Each module invokes a specific scheme tailored to its needs. In a given run a group of modules is selected to simulate a desired process. In some cases no recycle streams are present and one pass through each module will yield the desired result. On the other hand, it is very common for at least one recycle stream to be present. In this case iteration is required to reach the desired solution.

OSP iterates to a solution using simple functional iteration, as stream results are computed they are available for future computations. OSP continues computations, that is redoing calculations for each defined module, until an error criteria for the overall solution is met. The overall criteria is simply the maximum of the error from any module. Most modules have a defined error criteria based on the relative change between newly computed stream results and previously computed results. For all modules, except the ERROR module, these are based on normalized temperature changes. These error estimates are passed to the controller portion of OSP by each module. The user determines the overall error criteria by setting the TOL variable in the \$GENERAL input.

If the temperature is not deemed a sufficient criteria for convergence, or if for other reasons error results from a module will not lead to the desired measure of convergence, the ERROR module can be used. It allows criteria to be set on other aspects of the stream variables. The errors are defined based on the difference between stream values on the current and the immediately preceding computational loop.

The user should clearly understand that error as used here is only an error in the sense of an overall iteration scheme and is not an error for the single computational pass through the module. Modules signal OSP directly if they are unable to reach a satisfactory solution for a given set of input stream values.

OSP also provides a means of iterating on loops internal to the overall computational loop involving all defined modules. This is done by defining computational groups. A computational group should represent an internal recycle loop. It must be composed of modules which are contiguous in the overall computation scheme. The user can select up to 20 groups. Each group can have any number of members but the groups must not overlap. Group membership for a module is set by setting the GROUP variable in the module input section. Each computation group is executed a specified number of times on each overall loop iteration. The number of times to execute a group is set by the GROUP_LOOP parameter in the \$GENERAL input block. The user needs to be aware of the consequences of using internal loops on the error criteria set by individual modules. Since the individual modules do not distinguish between invocation as part of the overall loop iteration or an internal group iteration they may not set error criteria appropriate to control the overall iteration. This shortcoming can be overcome by using an ERROR module outside the loop to define error criteria for selected streams which will allow proper control of the overall iteration.

Criteria which determine the accuracy of the calculations for a given module is in general not available for alteration by the user. Criteria have been selected that insure sufficient precision of the solutions. Certain of the reaction modules are exceptions. The reaction modules all rely on routines which implement the plug-flow or well-mixed model. These routines in turn use the LSODE¹ software to perform the required numerical solutions. For the modules using the well-mixed model an error tolerance used by LSODE can be set by the user. This has been provided to allow solution of difficult systems to be accomplished, but also allows use of looser tolerances for easier problems. In general, the user should use default values of the tolerance parameter (RTOL) and only request tighter tolerances when computational problems are encountered.

RUNNING OSP

OSP is invoked by simply typing its name. Most of the input information comes from the ASCII input file, however there are several questions which are asked during startup which obtain their response from the standard input device.

The first question is

```
Input file name <end to end> ?
```

The response to this question should be the name of the ASCII input file. If the standard ".inp" suffix has been used in naming the suffix it may be omitted in the response, otherwise the full file name needs to be entered. Because of this default option an input file name must contain a period. If the run needs to be canceled, typing "end" will terminate it. If an error is made in typing the name and the file cannot be found, the above input prompt will be given again allowing another chance to correctly input the name.

The second question is

```
Root names for output files (def=X) ?
```

In the above the "x" will be set by the program to the name of the input file with the suffix (the last "." and anything beyond it) removed. A carriage return will use this name as the root name for the ".strm", ".dat" and ".mod" files.

The next series of questions is important if results present in a ".strm" file from a previous run are to be used. The first question of the series is

```
Initialize streams from file ? (def = n)
```

This is a "yes/no" question. The default is "no". OSP is asking if information from a previous ".strm" file is desired. If the response is "yes", then the internal stream data base will be initialized from the previous ".strm" file and only those streams not mentioned in that file will be defaulted to zero flow. The "yes" response brings the next question

```
Stream file name <end to end> ?
```

The name of the ".strm" file needs to be input. The suffix ".strm" is assumed. If the run needs to be canceled typing "end" will terminate it. Following this question is the inquiry about which snapshot of the stream information from the ".strm" file to use.

```
Loop and seq to get (.ge. 99 last) ?
```

Two numbers need to be input in response to this question, a loop number and a module sequence number. The ".strm" file can contain stream information from a previous run which was recorded after each module at each overall loop. Or it may contain only information about the streams after each overall computational loop. If the last set of stream information, presumably the results of successful completion of a previous run, are desired then two large numbers should be input, e.g. "99 99". If no loop or module with sequence numbers less than these values are present in the file the last entry is used. If information about the streams at some other point in the previous calculation is desired then the loop number and the module number of interest are

input. The stream information after execution of that module during the requested loop will be used. In any case a message is written to the standard output device and to the ASCII output file about which entry in the ".strm" file is used.

This completes the user input for the case of yes to the third question. It should be noted that information in \$INITSOLID, \$INITGAS and \$INITLIQ areas of the ASCII input file will overwrite information from the stream file. This turns out to be very useful when it is desired to redo a run with a very minor change in some stream variable.

If the response to the third question is "no", then the next inquiry from the program appears

```
Overwrite streams from file ? (def = n)
```

Again OSP is asking if information from a previous ".strm" file is desired. In this case information from the ".strm" file will overwrite information in the \$INITSOLID, \$INITGAS and \$INITLIQ areas of the ASCII input file. If the response is "yes", then the same set of questions as outlined just above will be used to request the name of the ".strm" file and the location within this file to obtain the stream data.

Two more questions which need response may follow. Whether they appear depends on details of the simulation and on control flags. The first of these is not optional and will appear if any reaction called for any a reaction module includes reactants not active in that module. The user is given a choice to proceed, however, generally the run should be terminated and the problem fixed. Comments on continuing with computations despite the warning are give below in the "Selection of Species and Reactions" section.

The final question which may appear is related to stream connections between modules. OSP determines the number of connections to modules for each stream. If any stream has an odd number of connections it may potentially indicate an error in setting up the input since in most cases streams leave one module and enter another. Of course for input and output streams for the overall process this is not the case and also for other reasons it may be desired to have used a given stream an odd number of times. OSP list the streams used an odd number of times and then gives the user the option to proceed or to terminate the run. If the simulation run is simple enough or if it has many unpaired streams the user may choose to turn off this warning/query by setting the \$GLOBAL parameter CHECK_CON to zero. It is defaulted to 1 which activates the connectivity check.

This completes direct interaction with the program. The user can cause the program to stop calculations at the end of a current computation loop and generate a ".dat" output file by creating a file with the name "break_file" under the same working directory as the shell executing the code. This is easily done on UNIX systems using the "touch" command.

During execution of the code a considerable amount of information about the course of calculations is generally written to the standard output device by the OSP control routines and by individual modules. It is often useful to use the UNIX I/O redirection commands to save this information in a file for later inspection.

THE TAB CODE

In addition to the basic OSP code there is a post processor code, TAB, available to the user. This code has a number of uses. It obtains stream information from a ".strm" file generated by OSP. It allows data to be extracted in a number of formats and printed either to the standard output device or an ASCII file.

User input as to the type of information requested is done through iteration with the standard input device. Three basic options are available: the "ge" option which will print stream information about all streams used in the computation at the end of a selected computational loop and module execution, the "sv" option which allow selected stream variables to be printed as a function of computational loop, and the "st" option which generates an output in a format suitable for use in the OSP input file for initializing stream variables (i.e. the \$INITOLID, \$INITGAS and \$INITLIQ sections of the ".inp" file).

REFERENCES

Thorsness, C.B. and Aldis, D. F., "Oil Shale Process Model (OSP) Theory Manual", *Lawrence Livermore National Laboratory UCRL-MA-119226*, 1994.

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Hindmarsh, A.C., "LSODE and LSODI, Two New Initial Value Ordinary Differential Equations Solvers', *ACS-Signum News 4 10* (1981).

APPENDIX A

THE "osp_input.doc" FILE

```
*****
***** DOCUMENTATION OF OSP INPUT PARAMETERS
(Rev 2.0)
*****
```

General comments:

The input file is arranged such that all input belongs to a named input group. A '\$' is used as a flag to indicate a group name is being defined. All input from one \$NAME (where NAME is the group names defined below) to the next \$NAME belongs to a given input group. A \$NAME can be repeated in the input file with the understanding that any conflicts will be resolved in favor of the last entry made in the input file. The exception to this is the \$MODULE groups which are used to define each new process module. Each occurrence is treated as a separate input group. The defined groups are:

\$GLOBAL - A limited number of control parameters.

\$PROPERTIES - Gas, solid and liquid species physical property parameters as well as reaction related parameters. Reaction parameters entered in this group generally serve to define default values for use in individual modules.

\$FLAGGAS - Set up gas use flags to be used in module definitions. This group name is followed by an "= NAME" where "NAME" is a name which is used for reference purposes. Name is up to 8 characters.

\$FLAGSOLID - Set up solid use flags to be used in module definitions. This group name is followed by an "= NAME" where "NAME" is a name which is used for reference purposes. Name is up to 8 characters.

\$FLAGLIQ - Set up liquid use flags to be used in module definitions. This group name is followed by an "= NAME" where "NAME" is a name which is used for reference purposes. Name is up to 8 characters.

\$FLAGREAC - Set up reaction use flags to be used in module definitions. This group name is followed by an "= NAME" where "NAME" is a name which is used for reference purposes. Name is up to 8 characters.

\$MODULE - Module definition group. Repeated for each module in the computation. This flag is followed by an "= TYPE" which defines the type of module selected.

\$INITGAS - Group used to initialize values of a gas stream. This flag is followed by an "= NAME" where "NAME" is the stream name of up to 8 characters.

\$INITLIQ - Group used to initialize values of a liquid stream. This flag is followed by an "= #" where "#" is the stream name of up to 8 characters.

\$INITSOLID - Group used to initialize values of a solid stream. This flag is followed by an "= #" where "#" is the stream name of up to 8 characters.

All input data is of the form NAME = value. All lines are parsed looking for equal signs as keys. The spaces are optional. Because of the rules used comment information can be used on the same line as data as long as it does not contain an equal sign. ASCII input containing blanks needs to be of the form 'string'. Any line

starting with a "*" is assumed to be a pure comment line and no input data parsing is performed.

In the following the name of the input parameter is given in at the start of each entry in capital letters. This is followed in brackets by the default value for the parameter and its units if appropriate. Following this is a description.

Note that the form of the default specifies the data type. In writing real numbers which are large or small the FORTRAN double precision notation "dnn is used, where "nn" is the desired power of ten. In some cases the values are defaulted in data statements. In this case the (data) is used and the appropriate data statement can be found below with the same name as the input parameter. In several cases the internal program name of the variable is not exactly the same as the input parameter name. In this case the name is added inside the brackets. Finally, in the case of the default stoichiometric factors, the values are given in a OSP subroutine. The code fragment in which they are defined is also given below. Species are sometimes defined by species number the correspondence between number and species is given in the data statement.

Defined below are:

```
* $GLOBAL  
* $PROPERTIES  
* $FLAGAS  
* $FLASOLID  
* $FLALIQ  
* $FLAGREAC  
* $MODULE  
* $INITGAS  
* $INITLIQ  
* $INITSOLID  
* Data statements which initialize species property variables (from props.f).  
* Code fragment which initializes stoichiometric coefficients for service  
routine kinetics (from subroutine setup_stoich in service.f).  
*****  
$GLOBAL  
*****
```

TITLE [' '] - A one line title for the problem.

LOOPMAX [100] - The maximum number of iterations around the complete computation loop allowed in the course of seeking a converged solution.

TOL [1.0d-3] - Fractional tolerance for a converged solution to overall problem.

CHECK_CON [1] - After reading all input data perform connectivity check before starting the computations. 1=yes, 0=no.

MODULO_ST [1] - The modulo of the computational loop for writing stream information to the binary output file.

CALC_WRITE [1] - Write module header information to TTY each time module called to perform a calculation. Also write module convergence error summary after each calculation loop. 1=write both types of information, 0=write only error summary, -1=write neither type of information.

ALL_MOD [0] - A flag which determines if stream data is written to the binary output file at the end of the full computational loop or at the end of each module computation: 0 = at the end of the computational loop, 1 = at the end of each module.

GROUP_LOOP(I) [1] - The loop parameter for the I'th module group (see GROUP in the universal parameters). The value determines the number of times a group of modules will be looped on during an overall computational loop. A value of one causes each member to be executed once. Since all modules are executed once regardless this parameter must have a value of two or greater to cause an internal computational loop to be executed. When internal loops are defined special consideration of error computations to determine convergence of the overall calculation may be required.

```
*****
$PROPERTIES
*****
```

Most the values in this section do not need to be modified from their default values. If the name change input is used then the \$PROPERTIES group shold proceed the \$MODULE and \$INIT- groups so that the changed names can be used in these groups.

<Generally Required Input>

SPHERICITY [1.0] - The sphericity parameter to use for solid particles.

<Solid>

SOLID_CPC(K,I) [data] - The K'th solid heat capacity coefficient for solid species I. Species heat capacity given by SOLID_CPC(1,I) + SOLID_CPC(2,I)*T + SOLID_CPC(3,I)*T**2 + SOLID_CPC(4,I)/T**2. The units are J/kg/K and T is the temperature in degrees K.

SOLID_HF(I) [data] - The heat of formation at 298 K in J/kg of solid species I.

SOLID_NAME(I) ['Name'] - The name of solid species I.

SOLID_WF_C(I) [data] - The weight fraction of organic carbon in solid species I.

SOLID_WF_C_IN(I) [data] - The weight fraction of inorganic carbon in solid species I.

SOLID_WF_H(I) [data] - The weight fraction of hydrogen in solid species I.

SOLID_WF_O(I) [data] - The weight fraction of oxygen in solid species I.

SOLID_WF_N(I) [data] - The weight fraction of nitrogen in solid species I.

SOLID_WF_S(I) [data] - The weight fraction of sulfur in solid species "I".

SOLID_RHO(I) [data] - The intrinsic density in kg/m**3 of solid species I.

<Gas>

GAS_CPC(K,I) [data] - The K'th gas heat capacity coefficient for gas species I. Species heat capacity given by GAS_CPC(1,I) + GAS_CPC(2,I)*T + GAS_CPC(3,I)*T**2. The units are J/mol/K and T is the temperature in degrees K.

GAS_HF(I) [data] - The heat of formation at 298 K in J/mol of gas species I.

GAS_C(I) [data] - The atoms of carbon per molecule of gas species I.

GAS_H(I) [data] - The atoms of hydrogen per molecule of gas species I.

GAS_O(I) [data] - The atoms of oxygen per molecule of gas species I.

GAS_N(I) [data] - The atoms of nitrogen per molecule of gas species I.

GAS_NAME(I) ['Name'] - The name of gas species I.

GAS_VISC(K,I) [data viscc] - The K'th gas viscosity coefficient for gas species I. Species viscosity given by GAS_VISC(1,I)*(T/273.0)**GAS_VISC(2,I). The units are kg/m/s and T is the temperature in degrees K.

GAS_MV(I) [data] - The molecular volume to use in the Fuller, Scheller and Giddings correlation for molecular diffusivities.

<Liquid>

LIQ_CPC(K,I) [data] - The K'th liquid heat capacity coefficient for liquid species I. Species heat capacity given by LIQ_CPC(1,I) + LIQ_CPC(2,I)*T + LIQ_CPC(3,I)*T**2. The units are J/kg/K and T is the temperature in degrees K.

LIQ_HF(I) [data] - The heat of formation at 298 K in J/kg of liquid species I.

LIQ_C(I) [data] - The atoms of carbon per molecule of liquid species I.

LIQ_H(I) [data] - The atoms of hydrogen per molecule of liquid species I.

LIQ_O(I) [data] - The atoms of oxygen per molecule of liquid species I.

LIQ_N(I) [data] - The atoms of nitrogen per molecule of liquid species I.

LIQ_NAME(I) ['Name'] - The name of liquid species I.

LIQ_S(I) [data] - The atoms of sulfur per molecule of liquid species I.

<Reaction Parameters>

REACTION_NAME(K) ['Name'] - The name of reaction K.

S_STOICH(I,K) [see stoich_setup] - Stoichiometric parameter for solid species I in reaction "K". The units are kg's of solid per unit of reaction. The unit of reaction is determined by the way the rate expression is formulated. This parameter can also be set by the STOICH module.

G_STOICH(I,K) [see stoich_setup] - Stoichiometric parameter for gas species I in reaction "K". The units are moles of gas per unit of reaction. The unit of reaction is determined by the way the rate expression is formulated. This parameter can also be set by the STOICH module.

L_STOICH(I,K) [see stoich_setup] - Stoichiometric parameter for liquid species I in reaction "K". The units are kg's of solid per unit of reaction. The unit of reaction is determined by the way the rate expression is formulated. This parameter can also be set by the STOICH module.

A_KER [2.81d13 1/s] - The pre-exponential factor in the kerogen decomposition reaction rate constant.

T_KER [26390.0 K]] - The activation temperature in the kerogen decomposition reaction rate constant.

DEO2_COEF [1.04d-15] - Factor used along with the original kerogen content to compute the effective oxygen diffusivity in pyrolyzed shale. The original kerogen content is obtained from solid stream variables.

A_CHAR_COMB [1.97d6 1/s] - The pre-exponential factor in the char combustion reaction rate constant.

T_CHAR_COMB [20202.0 K] - The activation temperature in the char combustion reaction rate constant.

A_COKE_COMB [1.97d6 1/s] - The pre-exponential factor in the coke combustion reaction rate constant.

T_COKE_COMB [20202.0 K] - The activation temperature in the coke combustion reaction rate constant.

DEL_COKE_COMB [0.105] - The fraction of a particle diameter to use in computing the mass transfer resistance internal to a particle used in the coke combustion rate model.

A_FES2_COMB [1.97d6 1/s] - The pre-exponential factor in the FeS2 combustion reaction rate constant.

T_FES2_COMB [20202.0 K] - The activation temperature in the FeS2 combustion reaction rate constant.

SOLID_INT [1.0d7 1/m] - The internal surface area of combusted shale. This parameter is used in the oil coking model.

NS_ADS [1.2d18 1/m**2] - The number of coking sites per unit internal area in combusted shale. This parameter is used in the coking model.

DEL_COKE [0.105] - The fraction of a particle diameter to use in computing the mass transfer resistance internal to a particle in the oil coking model.

COKE_RFAC [0.1] - The factor to multiply the mineral surface coking rate by to obtain the coking rate for that part of the surface already covered by coke.

A_COKE(K) [1.01d10 1/s] - The pre-exponential factor in the coking rate expression for oil component "K". "K" is 1, 2 or 3.

T_COKE(K) [19270.0 K] - The activation temperature in the coking rate expression for oil component "K". "K" is 1, 2 or 3.

A_ADS(K) [3.0d-7 Pa] - The pre-exponential factor in the oil adsorption equilibrium constant for oil component "K". "K" is 1, 2 or 3.

T_ADS(1) [4730.0 K] - The temperature in the exponential factor of the adsorption equilibrium constant for oil 1.

T_ADS(2) [6730.0 K] - The temperature in the exponential factor of the adsorption equilibrium constant for oil 2.

T_ADS(3) [7730.0 K] - The temperature in the exponential factor of the adsorption equilibrium constant for oil 3.

A_DOL(1) [4.08d7 1/s] - The pre-exponential factor in the MgCO3 decomposition reaction rate constant which is dominant in the absence of carbon dioxide.

T_DOL(1) [23320.0 K] - The activation temperature in the MgCO3 decomposition reaction rate constant which is dominant in the absence of carbon dioxide.

A_DOL(2) [9.02d4 1/s] - The pre-exponential factor in the MgCO3 decomposition reaction rate constant which is dominant in the presence of carbon dioxide.

T_DOL(2) [17010.0 K] - The activation temperature in the MgCO3 decomposition reaction rate constant which is dominant in the presence of carbon dioxide.

A_CAL(1) [1.3d10 1/s] - The pre-exponential factor in the CaCO₃ decomposition reaction rate constant which is dominant in the absence of carbon dioxide.

T_CAL(1) [27680.0 K] - The activation temperature in the CaCO₃ decomposition reaction rate constant which is dominant in the absence of carbon dioxide.

A_CAL(2) [5.60d8 1/s] - The pre-exponential factor in the CaCO₃ decomposition reaction rate constant which is dominant in the presence of carbon dioxide.

T_CAL(2) [29260.0 K] - The activation temperature in the CaCO₃ decomposition reaction rate constant which is dominant in the presence of carbon dioxide.

A_CAL(3) [8.52d12 1/s] - The pre-exponential factor in the CaCO₃ decomposition reaction rate constant involving silicon dioxide.

T_CAL(3) [40460.0 K] - The activation temperature in the CaCO₃ decomposition reaction rate constant involving silicon dioxide.

A_PCO2 [1.94d-13 Pa] - The pre-exponential factor in the carbon dioxide equilibrium relation used in the CaCO₃ decomposition rate model.

T_PCO2 [22360.0 K] - The temperature in the exponential factor in the carbon dioxide equilibrium reaction used in the CaCO₃ decomposition rate model.

A_EVAP(K) [1.0 1/s] - The scaling factor used to establish the evaporation rate of OIL-K, where K=1,2 or 3.

\$FLAGGAS = NAME

"NAME" [' '] - The name, up to 8 characters, of a group of gas species use flags. This name is used to reference the group when setting up modules.

GAS [' '] - The names of gas species to be included in a module. The input is repeated for each gas species needed. A list of gas names are given in the gas_name data statement below.

\$FLAGLIQ = NAME

"NAME" [' '] - The name, up to 8 characters, of a group of liquid species use flags. This name is used to reference the group when setting up modules.

LIQ [' '] - The names of liquid species to be included in a module. The input is repeated for each liquid species needed. A list of liquid names are given in the liq_name data statement below.

\$FLAGSOL = NAME

"NAME" [' '] - The name, up to 8 characters, of a group of solid species use flags. This name is used to reference the group when setting up modules.

SOL [' '] - The names of solid species to be included in a module. The input is repeated for each solid species needed. A list of solid names are given in the solid_name data statement below.

```
*****
$FLAGREAC = NAME
*****  
"NAME" [' '] - The name, up to 8 characters, of a group of reaction use flags. This name is used to reference the group when setting up modules.
```

```
REACTION [' '] - The names of reactions to be included in a module. The input is repeated for each reaction needed. A list of reaction names are given in the reaction_name data statement below.
```

```
*****
$MODULE = [See below for module name to use]
*****
```

General comments:

The order of module computation is the order in which modules are entered into the input file.

All modules have Universal Parameter input. Many have Block A Parameter input and some have Block B Parameter input.

Available modules:

ATTRITION	BALANCE	CNTR_CURRENT	CO_CURRENT	CSTR
ERROR	FLUID_BED	LIFT_PIPE	MERGE_STRMS	PACKED_BED
PASS_THRU	PHASE_CHANGE	PROP_TAB	RELAX	SPLIT_STRMS
STOICH	STOICH_REACT			

```
*****
Universal Parameters
*****
```

DESC [' '] - User description.

TAG [' '] - User tag up to 8 characters. Useful in logically grouping sets of modules. Not used by the code other than to label output.

GROUP [0] - Group number used to group modules for internal loops. The number should be between 1 & max_group (max_group=20). Groups cannot overlap and must be contiguous. The GROUP_LOOP global parameter is used to define the number of iterations desired.

```
*****
Block A Parameters (Basic setup parameters for reactor modules)
*****
```

<Stream Geometry>

GASIN [' '] - The name of the inlet gas stream.

GASOUT [' '] - The name of the outlet gas stream.

LIQIN [' '] - The name of the inlet liquid stream.

LIQOUT [' '] - The name of the outlet liquid stream.

SOLIDIN [' '] - The names of the solid inlet streams. Repeated for each solid inlet stream. The order defines the mapping to pairs of inlet/outlet solid streams used by other variables associated with solid streams (for example the solid use flags).

SOLIDOUT [' '] - The names of the solid outlet streams. Must be repeated as many times as SOLIDIN is repeated. The order sets the mapping from inlet to outlet streams to be used by the module.

<Species>

GAS [' '] - The names of gas species to be included in the module. The input is repeated for each gas species needed. A list of gas names are given in the `gas_name` data statement below.

GAS_FLAGS [' '] - The name of the block of gas species use flags to be used if desired. The name must have been defined in a `$FLAGGAS` block.

DEL_GAS [' '] - The names of gas species to be un-included in the module. The input is repeated for each gas species deleted. This is useful when a minor modification of a previously defined `$FLAGGAS` gas block is desired. The flags are processed in the order they appear in the input therefore the `DEL_GAS` parameter should follow the `GAS_FLAGS` parameter it is modifying.

LIQ [' '] - The names of liquid species to be included in the module. The input is repeated for each liquid species needed. A list of liquid names are given in the `liq_name` data statement below.

LIQ_FLAGS [' '] - The name of the block of liquid species use flags to be used if desired. The name must have been defined in a `$FLAGLIQ` block.

DEL_LIQ [' '] - The names of liquid species to be un-included in the module. The input is repeated for each liquid species deleted. This is useful when a minor modification of a previously defined `$FLAGLIQ` gas block is desired. The flags are processed in the order they appear in the input therefore the `DEL_LIQ` parameter should follow the `LIQ_FLAGS` parameter it is modifying.

SOLID(K) [' '] - The names of the solid species to be included in the module for the K'th solid stream. The input is repeated for each solid species needed. A list of solid names are given in the `solid_name` data statement below. The `SOLSAME` parameter can be used to reduce the required amount of input for cases in which a group of solid streams have the same species selected.

SOLSAME [0] - A parameter, which when set to 1, causes all the remaining solid streams in the module to use the same set of species as defined by the last explicitly set solid stream for the module. The total number of solid stream in/out pairs which require species flags to be set is established by the number of SOLIDIN's encountered. Since input data is processed as it is encountered in the file a `SOLSAME` will only load flags into the appropriate arrays up to the number of SOLIDIN's encountered before it in the module definition block. As a result it is usually best to declare all solid streams before using a `SOLSAME`.

SOL_FLAGS(K) [' '] - The name of the block of solid species use flags to be used for the K'th solid stream in the module. The name must have been defined in a `$FLAGSOLID` block.

DEL_SOL(K) [' '] - The names of liquid species to be un-included in the K'th solid stream in the module. The input is repeated for each solid species deleted. This is useful when a minor modification of a previously defined `$FLAGSOLID` solid block is desired. The flags are processed in the order they appear in the input therefore the `DEL_SOL` parameter should follow the `SOL_FLAGS` parameter it is modifying.

<Unit Geometry>

DIAM [0.0 m] - The effective diameter of the unit.

HEIGHT [0.0 m] - The effective height of the unit.

<Reaction Parameters>

REACTION [' '] - The names of the reactions which are to be used in the module. The input is repeated for each reaction selected. A list of reaction names is contained in the reaction_name data statement below.

REAC_FLAGS [' '] - The name of the block of reaction use flags to be used if desired. The name must have been defined in a \$FLAGREAC block.

DEL_REACTION [' '] - The names of reactions to be un-included in the module. The input is repeated for each reaction deleted. This is useful when a minor modification of a previously defined \$FLAGREAC block is desired. The flags are processed in the order they appear in the input therefore the DEL_REAC parameter should follow the REAC_FLAGS parameter it is modifying.

NS_ADS [\$PROPERTIES] - Overrides this parameter value set in the \$PROPERTIES group.

<Transport Parameters>

DEL_COKE [\$PROPERTIES] - Overrides this parameter value set in the \$PROPERTIES group.

DEL_COKE_COMB [\$PROPERTIES] - Overrides this parameter value set in the \$PROPERTIES group.

DIL_MV [17.9] - The molecular volume of the average bulk gas to be used in computing molecular diffusivities. The default is the appropriate value for nitrogen.

DIL_MW [0.028] - The molecular weight of the average bulk gas to be used in computing molecular diffusivities. The default is the appropriate value for nitrogen.

PRAN [0.7] - Gas Prandtl number used to compute gas thermal conductivity from viscosity and density data.

IBED [see modules] - Switch used in the calculation of gas to particle heat and mass transfer coefficients to determine whether packed bed or single particle correlations are used. 1 = single particle correlations, 2 = packed bed correlations.

IDILUTE [see modules] - Switch used in the calculation of gas to particle heat and mass transfer coefficients to determine if the effective particle diameter should be that of each individual solid stream or if a single area weighted particle diameter should be used in computing coefficients for all solid streams. 1 = individual particle diameter, 2 = single area weighted particle diameter. A value of 2 is usually best in dense phase systems.

<Miscellaneous>

DEBUG [1] - Flag to turn on extra intermediate output directed to standard out device. 1=on, 2=off.

Block B Parameters (Particle size distribution parameters for reactor modules)

PDIST_VF(I) [0.0] - Volume fraction of the I'th size class in the reactor. The size of this class is obtained from the input stream particle sizes provided by the mapping defined by the PDIST_STRM(I) input. The sum of the volume fractions must be one. The number of classes can run from one to the maximum number of reactor input solid streams. If this parameter and the PDIST_STRM parameter are completely omitted from the input then the size distribution in the reactor will be the same as that of the combined inlet solid streams and all particles will have the same residence time in the reactor.

PDIS_STRM(I) [' '] - The inlet stream associated with the I'th size class parameter, PDIST_VF(I). The parameter is repeated if more than one stream is to be associated with a prescribed PDIST_VF(I). Within a class the relative representation of each input stream in the reactor is determined by ratio of the input flow rates for those streams. If any PDIST_VF's are defined then all input streams must appear somewhere in a PDIS_STRM(I) input specification.

An example (a fragment of a definition of a CSTR module):

```

SOLIDIN = S1A  SOLIDIN=S1B  SOLIDIN=M1A  SOLIDIN=M1B

PDIST_VF(1)=0.75  PDIST_VF(1)=S1A  PDIST_VF(1)=M1A

PDIST_VF(2)=0.25  PDIST_VF(2)=S1A  PDIST_VF(2)=M1A

*****
$MODULE = ATTRITION
*****
```

This module performs attrition of solid particles. There are six attrition models which can be selected, TYPE 1, 2, 3, 4, 5, or 6. Input parameters are defined for each type of attrition.

Universal Parameters [See above] - Uses universal parameters.

----- TYPE = 1 -----

TYPE [1] - TYPE = 1 is the default type. This model allows a given particle size to be broken into "n" new particles the relative number of each new particle can be set. All new particles have the same composition as the input stream.

SI [0] - Input solid stream name.

SO(I) [0] - The I'th output stream name.

NEWDIAM(I) [0.0] - The diameter of the I'th output stream. If set to a negative number the particle will have the same size as the input stream.

SPLIT(I) [0] - The fraction of the input stream which is transformed into the I'th output stream (sum should be 1.0).

Sample Input: [type=1 si=10 so(1)=20 so(2)=21 so(3)=22 split(1)=0.1 split(2)=0.2 split(3)=0.7 newdiam(1)=0.003 newdiam(2)=0.002 newdiam(3)=0.001].

----- TYPE = 2 -----

TYPE [1] - The TYPE=2 model allows the attrition of partially burned particles to be modeled. An input stream is broken into two output streams. One consists of a particle containing all its carbon in its core surrounded by a depleted ash layer. The other particle stream contains only ash (i.e. no char). The carbon content of the core is obtained from solid stream variables.

SI [0] - Input solid stream name. The value of this streams PARAM_SOLID(1,N) solid stream variable defines the core carbon content.

SO(1) [0] - Carbon containing output stream name.

SO(2) [0] - Ash only output stream name.

ASHDIAM [0.0 m] - Diameter of the ash only particles.

ASHFRAC [0.0] - Fraction of the ash layer which forms new ash particles.

Sample Input: [type=2 si=10 si(1)=20 si(2)=21 ashdiam = 0.0001 m ashfrac=0.5].

----- TYPE = 3 -----

TYPE [1] - The TYPE = 3 model allows the attrition of partially burned particles to be modeled, with a fixed ash layer thickness. An input stream is broken into two output streams. One consists of a particle containing all of its carbon (char) in its core surrounded by a depleted ash layer which has a specified ash thickness. The other particle stream contains only ash (i.e. no char). The carbon content of the core is obtained from solid stream variables.

SI [0] - Input solid stream name. The value of this streams PARAM_SOLID(1,N) solid stream variable defines the core carbon content.

SO(1) [0] - Carbon containing output stream name.

SO(2) [0] - Ash only output stream name.

ASHDIAM [0.0 m] - Diameter of the ash only particles.

ASHTHICK [0.0 m] - Thickness of the remaining ash layer on the original particles. The new particle will have a diameter = core diameter + 2*ASHTHICK. A typical value is 0.2 d-3 m.

Sample Input: [type=3 si=10 si(1)=20 si(2)=21 ashdiam = 0.0001 m ashthick=0.2d-3].

----- TYPE = 4 -----

TYPE [1] - The TYPE=4 model allows the attrition of a particle to occur by reducing the size of the input particle and generating two output streams, one with a reduced size and the other (the attrited material) of a specified size. All output properties are the same as input properties with the exception of the diameter and the flow rate.

SI [0] - Input solid stream name.

SO(1) [0] - Reduced size particle output stream name.

SO(2) [0] - Attrited material output stream name.

SPLIT [0.0] - Fraction of the input material which is attrited.

NEWDIAM [0.0 m] - Diameter of the attrited particles.

Sample Input: [type=4 si=10 so(1)=20 so(2)=21 split=0.2 newdiam=0.00005]

----- TYPE = 5 -----

TYPE [1] - TYPE = 5 model is like the TYPE 1 model except that the new diameters are specified as a fraction of the source particle diameters rather than as an absolute size.

SI [0] - Input solid stream name.

SO(I) [0] - The I'th output stream name.

NEWDIAM(I) [0.0] - The diameter of the I'th output stream expressed as a fraction of the input solid particle diameters.

SPLIT(I) [0] - The fraction of the input stream which is transformed into the I'th output stream (sum should be 1.0).

```
Sample Input: [type=5 si=10 so(1)=20 so(2)=21 so(3)=22 split(1)=0.1 split(2)=0.2  
split(3)=0.7 newdiam(1)=0.5 newdiam(2)=0.2 newdiam(3)=0.1].
```

```
----- TYPE = 6 -----
```

TYPE [1] - The TYPE=6 model is the same as the TYPE 2 except the amount of removed material is set as a fraction of the total weight of the input stream and not as a fraction of the ash layer weight. The carbon content of the core is obtained from solid stream variables.

SI [0] - Input solid stream name. The value of this streams PARAM_SOLID(1,N) solid stream variable defines the core carbon content.

SO(1) [0] - Carbon enriched output stream name.

SO(2) [0] - Ash enriched output stream name.

ASHDIAM [0.0 m] - Diameter of the ash enriched particles.

SPLIT [0.0] - Fraction of the of the input mass to be split to the ash enriched stream.

```
Sample Input: [type=6 si=10 si(1)=20 si(2)=21 ashdiam = 0.0001 m split=0.5].
```

```
*****  
$MODULE = BALANCE  
*****
```

This module performs some overall balances using selected input and output streams. The balances included are atomic, energy and oil production/coking.

Universal Parameters [See above] - Uses universal parameters.

GI [' '] - Gas input stream name. May be repeated for multiple streams.

LI [' '] - Liquid input stream name. May be repeated for multiple streams.

SI [' '] - Solid input stream name. May be repeated for multiple streams.

GO [' '] - Gas output stream name. May be repeated for multiple streams.

LO [' '] - Liquid output stream name. May be repeated for multiple streams.

SO [' '] - Solid output stream name. May be repeated for multiple streams.

```
*****  
$MODULE = CNTR_CURRENT  
*****
```

This module allows a counter-current flow reactor to be modeled. The gas flow is counter current to the solids flow. The gas flow velocity is determined by reactor geometry parameters and the gas flow rate. The solid velocities for each solid stream are input parameters. These velocities and system geometry define the residence times. This module uses the internal well-mixed model to perform the actual calculations. The weighting factors for the well-mixed model are set so that the outlet composition and properties are used to determine the average reactor properties. To more accurately model a single real counter-current unit multiple CNTR_CURRENT computational units hooked in series should be used.

Universal Parameters [See above] - Uses universal parameters

Block A Parameters [See above] - Uses Block A parameters

IBED [2] - Heat transfer correlation flag defined in Block A parameters. Defaulted in this module to a packed-bed correlation.

IDILUTE [2] - Flag, defined in Block A parameters, used to set effective particle diameter used in gas to solid heat & mass transfer correlations. Defaulted in this module to use a single area weighted particle size for all streams.

EMISSIVITY [0.0] - Emissivity parameter for particle-to-wall radiation heat transport model.

VELP(K) [0.0 m/s] - Velocity of K'th solid stream where velocity is along the height dimension. The K'th solid is the K'th SOLID stream.

WEIGHT_GAS_IN [0.0] - Gas species weighting factor to use in the well-mixed model to arrive at average reactor composition. The average is given by WEIGHT_GAS_IN * (inlet gas property) + (1.0 - WEIGHT_GAS_IN) * (outlet gas property). Great care should be used when a value other than 0.0 is used since this may cause an inability to, find a solution.

WEIGHT_SOL_IN [0.0] - Solid species weighting factor to use in the well-mixed. Definition analogous to that for gases.

WEIGHT_LIQ_IN [0.0] - Liquid species weighting factor to use in the well-mixed. Definition analogous to that for gases.

```
*****  
$MODULE = CO_CURRENT  
*****
```

This module allows a dilute phase co-current plug-flow type reactor to be modeled. The gas and all solid streams may have seParame velocities. The liquid stream is given the velocity of the gas stream. This module uses the internal plug-flow model to perform the actual calculations.

Universal Parameters [See above] - Uses universal parameters

Block A Parameters [See above] - Uses Block A parameters

GAS_INIT [' '] - Stream name to use to initialize the inlet gas if temperature of GASIN stream is 0. This is useful to reduce the number of initial guesses required.

IBED [1] - Heat transfer correlation flag defined in Block A parameters. Defaulted in this module to a single-particle correlation.

IDILUTE [1] - Flag, defined in Block A parameters, used to set effective particle diameter used in gas to solid heat & mass transfer correlations. Defaulted in this module to use each solid stream's particle size.

HISTORY [' '] - Name to be given to an additional output file. If the name ends in .hst the output will be in hmp history file format. The data will be consist of dependent variable values as a function of position. If the name does not end in .hst the output will be as an ASCII table. The contents of the table will be <tab> delimited values of the temperatures as a function of position.

EMISSIVITY [0.0] - Emissivity parameter for particle-to-wall radiation heat transport model.

H LOSS [0.0 W/K/m**2] - Heat loss/gain coefficient defined for the reactor boundary. If given a value of -1 then the actual heat trasfer coefficient will be computed based on gas flow and correlations appropriate for flow inside a round conduit. If positive then then used as is for transport coefficient. Heat loss/gain from the system will be computed as H LOSS * DIAMETER * pi * dx * (tgas - T_AMBIENT) where tgas is the

local gas temperature, dx is a differential distance in the flow direction and T_AMBIENT is a sink/source (wall) temperature.

T_AMBIENT [0.0 K] - Sink/source (wall) temperature used in heat loss/gain calculation.

VELP(K) [0.0 m/s] - Velocity of K'th solid in the unit where motion is along the height dimension. The K'th solid is the K'th SOLID stream. A VELP must be specified for each solid stream pair defined in the module.

```
*****  
$MODULE = CSTR  
*****
```

This module allows a continuously fed stirred tank reactor(cstr) to be modeled. The residence time in the reactor is determined by solids and gas flow rates, reactor size, bed porosity, bed particle size distribution. This module uses the internal well-mixed model to perform the actual calculations. The weighting factors for the well mixed model are set so that the outlet composition and properties are used to determine the average reactor properties.

Universal Parameters [See above] - Uses universal parameters

Block A Parameters [See above] - Uses Block A parameters

Block B Parameters [See above] - Uses Block B parameters

GAS_INIT [' '] - Stream name to use to initialize the inlet gas if temperature of GASIN stream is 0. This is useful to reduce the number of initial guesses required.

IBED [1] - Heat transfer correlation flag defined in Block A parameters. Defaulted in this module to a single-particle correlation.

IDILUTE [2] - Flag, defined in Block A parameters, used to set effective particle diameter used in gas to solid heat & mass transfer correlations. Defaulted in this module to use a single area weighted particle size for allstreams.

RTOL [0.001] - Tolerance used in the solution scheme.

BEDP [0.6] - The void volume fraction. This includes gas filled space external to the solid particles.

WEIGHT_GAS_IN [0.0] - Gas species weighting factor to use in the well-mixed model to arrive at average reactor composition. The average is given by WEIGHT_GAS_IN * (inlet gas property) + (1.0 - WEIGHT_GAS_IN) * (outlet gas property). Great care should be used when a value other than 0.0 is used since this may cause an inability to, find a solution.

WEIGHT_SOL_IN [0.0] - Solid species weighting factor to use in the well-mixed. Definition analogous to that for gases.

WEIGHT_LIQ_IN [0.0] - Liquid species weighting factor to use in the well-mixed. Definition analogous to that for gases.

```
*****  
$MODULE = ERROR  
*****
```

ERROR allows the user to determine the iteration error for one or more streams. Several of the stream variables can be used in the error calculation, the flow rate, the temperature, and the species compositions. One or more of these variables can be used at one time. The individual errors are calculated as the difference in the

present iteration value and the last iteration value divided by the present value. All of the individual error results are averaged.

Universal Parameters [See above] - Uses universal parameters.

GI [' '] - Input gas stream name. Repeat for each stream.

GO [' '] - Output gas stream name. There should be one for each input.

LI [' '] - Input liquid stream name. Repeat for each stream.

LO [' '] - Output liquid stream name. There should be one for each input.

SI [' '] - Input solid stream name. Repeat for each input stream.

SO [' '] - Output solid stream name. There should be one for each input.

FLOW [0] - Flag if set to 1 will cause the stream flow rate to be included in the iteration error calculation.

TEMP [0] - Flag if set to 1 will cause the stream temperature to be included in the iteration error calculation.

DIAM [0] - Flag if set to 1 will cause the solid stream diameters to be included in the iteration error calculation.

GAS [' '] - The names of gas species to be included in the error calculation. The input is repeated for each gas species needed. A list of gas names are given in the gas_name data statement below.

LIQ [' '] - The names of liquid species to be included in the error calculation. The input is repeated for each liquid species needed. A list of liquid names are given in the liq_name data statement below.

SOL [' '] - The names of solid species to be included in the error calculation. The input is repeated for each solid species needed. A list of solid names are given in the solid_name data statement below.

```
*****  
$MODULE = FLUID_BED  
*****
```

This module allows a fluid bed reactor with an emulsion phase and a bubble phase to be modeled. The residence time in the reactor is determined by solids and gas flow rates, reactor size, bed porosity and bed particle size distribution. The size of bubbles, the exchange rates between bubbles and emulsion phases and degree of discretization of the bubble phase are controlled by input parameters.

Universal Parameters [See above] - Uses universal parameters.

Block A Parameters [See above] - Uses Block A parameters.

Block B Parameters [See above] - Uses Block B parameters.

GAS_INIT [' '] - Stream name to use to initialize the inlet gas if temperature of GASIN stream is 0. This is useful to reduce the number of initial guesses required.

NBUB [1] - Number of axial divisions for bubble phase.

B_FB [' '] - Name of the stream to hold information on the internal bubble stream. One is needed for each bubble. If not explicitly assigned the code will automatically assign a unique name.

DB_COEF [0.00853] - Coefficient for bubble size correlation.
 UB_COEF [0.771] - Coefficient for bubble velocity correlation.
 QDOT_COEF [4.675d-2] - Coefficient for bubble-emulsion exchange correlation.
 C1 [0.5] - Parameter for fb, bubble fraction-limit calculation. Below this value no limit correction is applied.
 C2 [0.74] - Parameter for fb, bubble fraction-limit calculation. This is the maximum bubble fraction allowed in the limit calculation.
 C3 [10.] - Parameter for fb, bubble fraction-limit calculation. If fb initially had a value C3, it would have a value of C4 after the limit calculation.
 C4 [0.73] - Parameter for fb, bubble fraction-limit calculation. If fb initially had a value C3, it would have a value of C4 after the limit calculation.
 RTOL [0.001] - Tolerance used in the solution scheme.
 BEDP [0.6] - The void fraction of the emulsion phase.
 DP_SCALE [1.0] - A multiplicative factor which converts stream particle diameters to an effective values for use in fluidization correlations. A single factor is applied to all particles in the module.
 WEIGHT_GAS_IN [0.0] - Gas species weighting factor to use in the well-mixed model to arrive at average reactor composition. The average is given by WEIGHT_GAS_IN * (inlet gas property) + (1.0 - WEIGHT_GAS_IN) * (outlet gas property). Great care should be used when a value other than 0.0 is used since this may cause an inability to, find a solution.
 WEIGHT_SOL_IN [0.0] - Solid species weighting factor to use in the well-mixed. Definition analogous to that for gases.
 WEIGHT_LIQ_IN [0.0] - Liquid species weighting factor to use in the well-mixed. Definition analogous to that for gases.

```
*****
$MODULE = LIFT_PIPE
*****
```

This module allows a dilute phase lift pipe to be modeled. The gas and all solid streams may have seParame velocities. The solid velocities are obtained from input slip velocities or an internal slip velocity model. This module uses the internal plug-flow model to perform the actual calculations. An optional history file may be written to obtain results at intermediate heights.

Universal Parameters [See above] - Uses universal parameters.
 Block A Parameters [See above] - Uses Block A parameters. Except liquids are not used in this module.
 IBED [1] - Heat transfer correlation flag defined in Block A parameters. Defaulted in this module to a single particle correlation.
 IDILUTE [1] - Flag, defined in Block A parameters, used to set effective particle diameter used in gas to solid heat & mass transfer correlations. Defaulted in this module to use each solid stream's particle size.
 HISTORY [' '] - Name to be given to a optional output file. If the name ends in .hst the output will be in hmp history file format. The data will be output of dependent variable values as a function of position. If the name does not end in .hst the

output will be as an ASCII table. The contents of the table will be <tab> delimited values of the temperatures as a function of position.

EMISSIVITY [0.0] - Emissivity parameter for particle-to-wall radiation heat transport model.

VSLIP(K) [0.0 m/s] - Slip velocity of K'th solid in the unit where motion is along the height dimension. Used if VSLIPCALC=0. The K'th solid is the K'th SOLIDIN.

VSLIPCALC [1] - Flag to determine whether the solid-gas slip velocities are computed internally or if input values are used. 0 = use input values, 1 = calculate internally. The K'th solid is the K'th SOLIDIN.

H_LOSS [0.0 W/K/m**2] - Heat loss/gain coefficient defined for the reactor boundary. If given a value of -1 then the actual heat transfer coefficient will be computed based on gas flow and correlations appropriate for flow inside a round conduit. If positive then used as is for transport coefficient. Heat loss/gain from the system will be computed as H_LOSS * DIAMETER * pi * dx * (tgas - T_AMBIENT) where tgas is the local gas temperature, dx is a differential distance in the flow direction and T_AMBIENT is a sink/source (wall) temperature.

T_AMBIENT [0.0 K] - Sink/source (wall) temperature used in heat loss/gain calculation.

CWIN [0.03] - Solid-wall friction coefficient, used if VSLIPCALC=1.

ANUIN [2.] - Coefficient of restitution term, used if VSLIPCALC=1.

ICYCMAXIN [10000] - Maximum number of iterations to be allowed in internal slip velocity calculations, used if VSLIPCALC=1.

DTIN [0.001] - Cycle step size, used if VSLIPCALC=1.

```
*****
$MODULE = MERGE_STRMS
*****
```

This module combines multiple input streams into a smaller number of output streams. All output streams are in thermal equilibrium. The outlet temperature is determined by adiabatic mixing of all input streams in the absence of any reactions. Only one oil and gas stream can leave the module but multiple solid streams can be defined by specifying group membership as described below.

Universal Parameters [See above] - Uses universal parameters.

PRINT [1] - Flag which indicates if module results are to be printed [0=no, 1=yes].

GI [' '] - Input gas stream name. Repeat for each stream.

GO [' '] - Output gas stream name. There should be only one.

LI [' '] - Input liquid stream name. Repeat for each stream.

LO [' '] - Output liquid stream name. There should be only one.

SI(K) [' '] - Input solid stream name for the K'th solid stream group. Repeat for each input stream for the group.

SO(K) [' '] - Output solid stream name for the K'th solid stream group. There should be only one SO for each group.

HEAT [0.0 W] - Heat load, positive represents heating of streams.

```
*****  
$MODULE = PACKED_BED  
*****
```

This module allows a dense phase co-current plug flow type reactor to be modeled. (The CO_CURRENT, or LIFT_PIPE modules should be used for dilute phase systems.) The residence time of material is defined by the bed porosity, overall flow rates and reactor geometry. The internal plug-flow module is used to perform the actual calculations.

Universal Parameters [See above] - Uses universal parameters.

Block A Parameters [See above] - Uses Block A parameters. Except liquids are not used in this module.

IBED [2] - Heat transfer correlation flag defined in Block A parameters. Defaulted in this module to a packed-bed correlation.

IDILUTE [2] - Flag, defined in Block A parameters, used to set effective particle diameter used in gas to solid heat & mass transfer correlations. Defaulted in this module to use a single area weighted particle size for all streams.

BEDP [0.4] - The void fraction of the bed. This includes gas phase volume in the emulsion phase and the bubble volume.

```
*****  
$MODULE = PASS_THRU  
*****
```

This module allows a stream to be renamed. The module passes the stream information from the input stream to the output stream with no change.

Universal Parameters [See above] - Uses universal parameters.

GI [' '] - Input gas stream name. Repeat for each stream.

GO [' '] - Output gas stream name. There should be one for each input.

LI [' '] - Input liquid stream name. Repeat for each stream.

LO [' '] - Output liquid stream name. There should be one for each input.

SI [' '] - Input solid stream name. Repeat for each input stream.

SO [' '] - Output solid stream name. There should be one for each input.

```
*****  
$MODULE = PHASE_CHANGE  
*****
```

This module allows phase changes between liquid and gas to be accomplished. Simple, material balance based algorithms are used, no phase equilibrium considerations are included.

Universal Parameters [See above] - Uses universal parameters.

TYPE [' '] - Type of phase change required, 'C' for condensation and 'E' for evaporation.

----- TYPE = 'C' -----

The condensation mode allows selected components to be condensed from the gas phase to the liquid phase. Gas species which can undergo condensation have a non-zero value of the GAS_TO_LIQ parameter defined in the other_props common and are initialized in the block data section at the end of the props.f file. In this mode one gas input stream is required. Each condensed species is put into a separate liquid stream specified by the user.

GI [' '] - Gas input stream name, must have one and only one.

GO [' '] - Gas output stream name, must have one and only one.

LO [' '] - Liquid output stream name. Must be repeated for each species condensed. The order of input ties it to the corresponding species defined by GAS.

GAS [' '] - Name of the gas species to condense. Repeat for each species that is to be condensed.

TEMP [0.0 K] - If set then outlet streams temperature. If not set then outlet streams will have the same temperature as the inlet gas streams.

PRES [0.0 Pa] - If set then outlet gas stream pressure. If not set then outlet gas stream will have the same pressure as the inlet gas streams.

----- TYPE = 'E' -----

The evaporation mode allows selected components to be evaporated from the the liquid phase to the gas phase. All liquid species can undergo evaporation. In this mode one liquid input stream is required. A gas input stream is optional.

GI [' '] - Gas input stream name, optional.

GO [' '] - Gas output stream name, must have one and only one.

LI [' '] - Liquid input stream name, must have one and only one.

LO [' '] - Liquid input stream name, must have one and only one.

LIQ [' '] - Name of the liquid species to evaporate. Repeat for each species that is to be evaporated.

TEMP [0.0 K] - If set then outlet streams temperature. If not set then outlet streams will have the same temperature as the inlet gas streams. If no gas inlet stream has been declared this parameter must be set.

PRES [0.0 Pa] - If set then outlet gas stream pressure. If not set then outlet gas stream will have the same pressure as the inlet gas streams. If no gas inlet stream has been declared this parameter must be set.

\$MODULE = PROP_TAB

This modules allows a table to be output which contains all of the pure species properties over a selected range of temperatures. Optionally mixture properties can also be obtained.

Universal Parameters [See above] - Uses universal parameters.

TMAX [0.0 K] - Upper temperature.

TMIN [0.0 K] - Lower temperature.
 DT [0.0 K] - Temperature step.
 GS [' '] - Optional gas stream name to used to compute mixture properties.
 SS [' '] - Optional solid stream name used to compute mixture properties.
 LS [' '] - Optional liquid stream name used to compute mixture properties.

\$MODULE = RELAX

This module allows solid stream updating which blends old and new values of stream parameters. A choice of which solid properties are relaxed is provided through an input parameter. This relaxation to newly computed values is sometimes necessary to allow the steady-state condition of a recycle loop to be reached without going into oscillations.

Universal Parameters [See above] - Uses universal parameters.

PRINT [1] - Flag which determines if module results are printed, 0 = no, 1 = yes.

SOLIDIN [' '] - Stream name of input solid stream. Repeated for each input stream.

SOLIDOUT [' '] - Stream name of output solid stream. Repeated for each output stream. The order maps the input streams to the output streams.

RELAX [0.5] - Relaxation factor to use. Updated stream variables will be set to RELAX times new values plus [1-RELAX] times old values.

FLAG ['AL'] - Type of relaxation: 'AL' - all solid properties, 'TE' - temperature only, 'NT' - all properties except temperature.

COUNTER [1] - Counter which determines when relaxation starts. Normally relaxation is applied only after one computation loop. This is because no valid old values have been calculated. However, on a restart it may be that relaxation is desired on first computation loop. If this is the case COUNTER should be set to 2.

\$MODULE = SPLIT_STRMS

This module allows a single gas, liquid and/or solid stream to be split into two output streams. The splitting can be done on a fractional bases or an absolute flow rate level can be specified for one outlet stream with the other carrying the remainder of the flow. It is also possible to use this module to multiply a stream flow by any real value. This is accomplished by defining only one output stream and setting the split factor to the desired multiplier. Note the split parameters means flow if positive and fraction if negative. Split applies to the first defined output stream, the second gets the leftover.

Universal Parameters [See above] - Uses universal parameters.

PRINT [1] - Flag which determines whether the module results are printed, 0 = no, 1 = yes.

GI [' '] - Gas input stream name, only one.

GO [' '] - Gas output stream name. Except when a simple multiplication is desired there should be two GO streams.

GSPLIT [0.0] - This parameter defines the type of manipulation to be done. If positive the value is interpreted as an absolute flow. The flow of the first GO stream is set to GSPLIT and the remaining flow is placed in the second GO stream. If the parameter is negative then it is interpreted as a multiplier. For true splitting the value should be a number between 0 and 1. In this case the first GO stream is given GSPLIT of the flow and the second GO stream is given [1- GSPLIT] of the flow. If only one GO stream is defined then the input flow is simply multiplied by GSPLIT and placed in the output stream.

LI [' '] - Liquid input stream name, only one.

LO [' '] - Liquid output stream name. Except when a simple multiplication is desired there should be two LO streams.

LSPLIT [0.0] - Definition equivalent to that of GSPLIT above except flow rate is in kg/s.

SI [' '] - Solid input stream name. This may be repeated so that multiple solid streams can be handled.

SO(I) [' '] - Solid output stream name. The index I is either 1 or 2 indicating if this is the 1st or 2nd stream. This is required to help in the bookkeeping for the solid streams. The SI and SO's are linked together by the order in which they appear.

SSPLIT [0.0] - Definition equivalent to that of GSPLIT above except flow rate is in kg/s. Only one value is allowed. It is applied to all solid groups.

\$MODULE = STOICH

This module allows reaction stoichiometry to be computed from input material balance information. The module also computes and outputs heats of reaction over a selected temperature range. Input material balance information are obtained from selected input stream information. In general it is probably best just to set stream flows to 1 and then treat composition variables as quantities. For this purpose negative composition variables are OK and should be used to represent reactants. Note all streams used must have a flow rate, therefore streams which only have computed results still need to be initialized with a flow of one. This module can be used alone to allow stoichiometric and heats of reaction information to be output or optionally it can reset internal stoichiometric coefficients for a selected reaction which then can be used by other modules.

Universal Parameters [See above] - Uses universal parameters

TMAX [0.0 K] - Upper temperature.

TMIN [0.0 K] - Lower temperature.

DT [0.0 K] - Temperature step.

GS [' '] - Gas stream name. (Note: Gases are in moles.)

SS [' '] - Solid stream name. (Note: Solids are in kg's.)

LS [' '] - Oil stream name. (Note: Liquids are in kg's.)

GAS [' '] - Name of gas whose stoichiometric coefficient is desired. Repeat for each gases desired.

SOL [' '] - Name of solid whose stoichiometric coefficient is desired. Repeat for each solid desired.

LIQ [' '] - Name of liquid whose stoichiometric coefficient is desired. Repeat for each liquid desired.

G_BASE [' '] - Name of gas that is to have a stoichiometric coefficient of one.

S_BASE [' '] - Name of solid that is to have a stoichiometric coefficient of one.

L_BASE [' '] - Name of liquid that is to have a stoichiometric coefficient of one.

C_BAL [0] - Set to one if carbon balance desired.

H_BAL [0] - Set to one if hydrogen balance desired.

O_BAL [0] - Set to one if oxygen balance desired.

N_BAL [0] - Set to one if nitrogen balance desired.

S_BAL [0] - Set to one if sulfur balance desired.

SET_REACT [0] - The reaction number for which the stoichiometric coefficients just determined are to be set. This overrides hardwired coefficients. If zero then reaction stoichiometry is only printed to the output file and no internal reaction coefficients are set.

```
*****
$MODULE = STOICH_REACT
*****
```

This module models a stoichiometric reactor. The extent off reaction is specified by stoichiometric fractions based on input reactants. One input gas and one liquid stream are considered, but multiple input solid streams are handled. Since stoichiometry is done relative to inlet amounts two step proccesses require the use of multiple modules (e.g. coking of gas phase oil). Also it is possible to require more than the available amount of a reactant to be consumed if it is consumed by more than one reaction. If this occurs an error message is reported and calculations are terminated. Outlet temperatures can be computed based on adiabatic operation (with the possible addition or subtraction of a specified amount of heat), or by setting the outlet temperatures. In the later case the heat gain/loss is computed.

Universal Parameters [See above] - Uses universal parameters.

TYPE [1] - Type of calculation to perform. 1 = adiabatic mode, 2 = outlet temperature set

GASIN [' '] - The name of the inlet gas stream.

GASOUT [' '] - The name of the inlet gas stream.

LIQIN [' '] - The name of the inlet liquid stream.

LIQOUT [' '] - The name of the inlet liquid stream.

SOLIDIN [' '] - The names of the solid inlet streams. Repeated for each solid inlet stream.

SOLIDOUT [' '] - The names of the solid outlet streams. Must be repeated as many times as SOLIDIN is repeated.

REACTION [' '] - The names of the reactions to consider. Repeated for each reaction desired. The input order defines the input order for the corresponding ST_REAC.

ST_REAC [0.0] - The extent of the corresponding reaction. Based on stoichiometry as given by OSP stoichiometric coefficients and the input flow rates of involved species.

----- TYPE = '1' -----

All output temperatures are equal and are computed assuming adibatic operation which includes an option heat source/sink parameter.

HEAT [0.0 W] - Optional heat load, positive represents heating of streams.

----- TYPE = '2' -----

Output temperatures are set by input parameters. Heat source/sink is computed.

TEMP_GAS [0.0 K] - The temperature of the gas outlet stream.

TEMP_SOL [0.0 K] - The temperature of the solid outlet stream(s).

TEMP_LIQ [0.0 K] - The temperature of the liquid outlet stream.

\$INITGAS = STREAM-NAME

"STREAM NAME" - Name of the gas stream to initialize.

FLOW [0.0 mol/sec] - Molar flow rate of gas stream.

TEMP [0.0 K] - Temperature of gas stream.

PRES [0.0 Pa] - Pressure of gas in stream.

"NAME" [' '] - Mole fraction of stream gas species with name "NAME", for example: o2 = 0.21 would assign the mole fraction of o2 in the gas stream a value of 0.21.

SAME_AS [' '] - Set this streams property values to that of the stream named. The named stream should have been previously initialized. The position of the SAME_AS declaration in the input is important since at the point it is detected in the left-to-right top-to-bottom decoding of the input information all variables are set to those of the declared stream. Any other declarations of variables after this point overwrites these values. In this way, for example, if one wants a given stream to have the same properties as stream 'GAS_INPUT' except for flow rate one would use:
\$INITGAS=NEWGAS SAME_AS='GAS_INPUT' FLOW=1.25

\$INITLIQ = STREAM-NAME

"STREAM NAME" - Name of the liquid stream to initialize.

FLOW [0.0 kg/sec] - Mass flow rate of the liquid stream.

TEMP [0.0 K] - Temperature of the liquid stream.

"NAME" [0.0] - Mass fraction of stream liquid species with name "NAME", for example: oil-1 = 0.1 would assign the mass fraction of oil-1 in the liquid stream a value of 0.1.

SAME_AS [' '] - Set all values to those of the specified stream. See \$INITGAS for detailed description.

```
*****
$INITOLID = STREAM-NAME
*****

"STREAM-NAME" - Name of the solid stream to initialize.

FLOW [0.0 kg/sec] - Mass flow rate of the solid stream.

TEMP [0.0 K] - Temperature of the solid stream.

DIAM [0.0 m] - Diameter of particles in the solid stream.

POR [0.0] - Porosity of the particles in the solid in stream.

"NAME" [0.0] - Mass fraction of stream solid species with name "NAME", for example:
kerogen-1 = 0.1 would assign the mass fraction of kerogen-1 in the solid stream a
value of 0.1.

PROP(1) [0.0 kg/m**3] - Auxiliary solid property 1 which is defined as the original
char content of the stream. This property is used in attrition and char combustion
models. The char content should include all components and should be expressed as an
absolute density (i.e. kg of char per cubic meter of particle).

PROP(2) [0.0 kg/m**3] - Auxiliary solid property 2 which is defined as the original
kerogen content of the stream. This property is used in the combustion models to
compute effective oxygen diffusivity in a particle. The kerogen content should be
expressed as an absolute density (i.e. kg of kerogen per cubic meter of particle).

PROP(3) [0.0 kg/m**3] - Auxiliary solid property 3 which is defined as the original
FeS2 content of the stream. This property is used in FeS2 combustion model. The FeS2
should be expressed as an absolute density (i.e. kg of FeS2 per cubic meter of
particle).

SAME_AS [' '] - Set all values to those of the specified stream. See $INITGAS for
detailed description.

*****
Data statements from the props.f file.
*****
```

C		
C	gas names	
	data gas_name/	
C	-----1. -----	-----2. -----
&	'N2 ',	'O2 ',
C	-----3. -----	-----4. -----
&	'H2 ',	'CO ',
C	-----5. ---	-----6. H2O -----
&	'CO2 ',	'H2O ',
C	-----7. -----	-----8. SO2 -----
&	'H2S ',	'SO2 ',
C	-----9. -----	-----10. NO2 -----
&	'NH3 ',	'NO2 ',
C	-----11. -----	-----12. -----
&	'HCN ',	'COS ',
C	-----13. -----	-----14. -----
&	'CH4 ',	'C2H4 ',
C	-----15. -----	-----16. -----
&	'C2H6 ',	'C3H6 ',
C	-----17. -----	-----18. -----
&	'C3H8 ',	'C5-pseudo ',
C	-----19. -----	-----20. -----
&	'H12-pseudo ',	'Oil-1 ',

```

c      -----21. -----
c          &           'Oil-2      ', -----22. -----
c      -----23. -----
c          &           'Oil-4      ', -----24. -----
c      -----25. -----
c          &           'Gas-A      ', -----26. -----
c      -----27. -----
c          &           'Gas-C      ', -----28. -----
c                           'Gas-D      '/

c solid names
  data solid_name/
c      -----1. -----
c          &           'Kerogen-1   ', -----2. -----
c      -----3. -----
c          &           'Kerogen-3   ', -----4. -----
c      -----5. -----
c          &           'Char-H     ', -----6. -----
c      -----7. -----
c          &           'Char-N     ', -----8. -----
c      -----9. -----
c          &           'Inert      ', -----10. -----
c      -----11. -----
c          &           'Bound-water ', -----12. -----
c      -----13. -----
c          &           'CaO        ', -----13. -----
c      -----15. -----
c          &           'MgCO3      ', -----14. -----
c      -----17. -----
c          &           'MgSO4      ', -----15. -----
c      -----19. -----
c          &           'FeS2       ', -----16. -----
c      -----21. -----
c          &           'Fe2O3      ', -----17. -----
c      -----23. -----
c          &           'N-inorganic ', -----18. -----
c      -----25. -----
c          &           'Oil-2      ', -----19. -----
c      -----27. -----
c          &           'Oil-4      ', -----20. -----
c      -----29. -----
c          &           'Coke       ', -----21. -----
c      -----31. -----
c          &           'Solid-A    ', -----22. -----
c      -----33. -----
c          &           'Solid-C    ', -----23. -----
c                           'Solid-D    '/

c liq names
  data liq_name/
c      -----1. -----
c          &           'Oil-1      ', -----2. -----
c      -----3. -----
c          &           'Oil-3      ', -----4. -----
c      -----5. -----
c          &           'Oil-5      ', -----6. -----
c      -----7. -----
c          &           'Liquid-A   ', -----8. -----
c                           'Liquid-B  '/

c liq to gas map
  data liq_to_gas_map/
c      -----1. Oil-1 -----2. Oil-2 -----
c          20,           21,
c      -----3. Oil-3 -----4. Oil-4 -----
c          22,           23,
c      -----5. Oil-5 -----6. Water -----

```

```

&          24,
c      -----7. Liquid-A -----       6 ,  

&          25,                   8. Liquid-B -----  

&                               26 /  

c  gas to liquid map
  data gas_to_liq_map/
    &-----1. N2 ----- 2. O2 -----
    &          0,          0,  

    &-----3. H2 ----- 4. CO -----
    &          0,          0,  

    &-----5. CO2 ----- 6. H2O -----
    &          0,          6,  

    &-----7. H2S ----- 8. SO2 -----
    &          0,          0,  

    &-----9. NH3 ----- 10. NO2 -----
    &          0,          0,  

    &-----11. HCN ----- 12. COS -----
    &          0,          0,  

    &-----13. CH4 ----- 14. C2H4 -----
    &          0,          0,  

    &-----15. C2H6 ----- 16. C3H6 -----
    &          0,          0,  

    &-----17. C3H8 ----- 18. C5 (1/2*C5H12)
    &          0,          0,  

    &-----19. H12 ----- 20. Oil-1 -----
    &          0,          1,  

    &-----21. Oil-2 ----- 22. Oil-3 -----
    &          2,          3,  

    &-----23. Oil-4 ???----- 24. Oil-5 -----
    &          4,          5,  

    &-----25. Gas-A ----- 26. Gas-A -----
    &          7,          8,  

    &-----27. Gas-C ----- 28. Gas-D -----
    &          0,          0 /  

c  gas heats of formation at 298.15 K in J/mol
  data gas_hf/
    &-----1. N2 ----- 2. O2 -----
    &          0.0,          0.0,  

    &-----3. H2 ----- 4. CO -----
    &          0.0, -1.1052d5,  

    &-----5. CO2 ----- 6. H2O -----
    &          -3.9351d5, -2.4183d5,  

    &-----7. H2S ----- 8. SO2 -----
    &          -2.0146d4, -2.9690d5,  

    &-----9. NH3 ----- 10. NO2 -----
    &          -4.6191d4, 3.3644d4,  

    &-----11. HCN ----- 12. COS ???-----
    &          -1.3d5, -99.0,  

    &-----13. CH4 ----- 14. C2H4 -----
    &          -7.4848d4, 5.2283d4,  

    &-----15. C2H6 ----- 16. C3H6 -----
    &          -8.4667d4, 2.0413d4,  

    &-----17. C3H8 ----- 18. C5 (1/2*C5H12)
    &          -1.0385d5, -8.3596d4,  

    &-----19. H12 ----- 20. Oil-1 -----
    &          -8.3596d4, -2.69d5,  

    &-----21. Oil-2 ----- 22. Oil-3 -----
    &          -5.37d5, -7.01d5,  

    &-----23. Oil-4 ----- 24. Oil-5 -----
    &          0.0, 0.0,  

    &-----25. Gas-A ----- 26. Gas-B -----
    &          0.0, 0.0,

```

```

c      -----27. Gas-C -----      -----28. Gas-D -----
c      &          0.0,                  0.0/
c
c
c  gas heat capacities. a + bT + cT**2  J/K/mol
  data gas_cpc/
    -----1. N2 -----      -----2. O2 -----
    & 27.30, 5.230d-3, -4.184d-9, 25.72, 1.298d-2, -3.863d-6,
    -----3. H2 -----      -----4. CO -----
    & 29.07, -8.368d-4, 2.013d-6, 26.86, 6.966d-3, -8.201d-7,
    -----5. CO2 -----      -----6. H2O -----
    & 26.00, 4.350d-2, -1.483d-5, 30.36, 9.615d-3, 1.184d-6,
    -----7. H2S -----      -----8. SO2 -----
    & 27.87, 2.148d-2, -3.573d-6, 29.77, 3.980d-2, 1.469d-5,
    -----9. NH3 -----      -----10. NO2 ??? -----
    & 25.46, 3.687d-2, -6.301d-6, 30.00, 0.0, 0.0,
    -----11. HCN ???-----      -----12. COS ???-----
    & 30.00, 0.0, 0.0, 30.00, 0.0, 0.0,
    -----13. CH4 -----      -----14. C2H4 -----
    & 14.15, 7.550d-2, -1.799d-5, 11.84, 1.197d-1, -3.651d-5,
    -----15. C2H6 -----      -----16. C3H6 -----
    & 9.40, 1.598d-1, -4.623d-5, 13.61, 1.888d-1, -5.749d-5,
    -----17. C3H8 -----      -----18. C5 -----
    & 10.08, 2.393d-1, -7.336d-5, 10.24, 1.885d-1, -5.866d-5,
    -----19. H12 -----      -----20. Oil-1 -----
    & 10.24, 1.885d-1, -5.866d-5, 47.7, 7.9d-1, 2.58d-4,
    -----21. Oil-2 -----      -----22. Oil-3 -----
    & 107.2, 1.7, 5.5d-4, 143.8, 2.25d-1, 7.18d-4,
    -----23. Oil-4 ???-----      -----24. Oil-5 ???-----
    & 600.0, 0.0, 0.0, 600.0, 0.0, 0.0,
    -----25. Gas-A -----      -----26. Gas-B -----
    & 30.0, 0.0, 0.0, 30.0, 0.0, 0.0,
    -----27. Gas-C -----      -----28. Gas-D -----
    & 30.0, 0.0, 0.0, 30.0, 0.0, 0.0/
c
c  solid heat of formation at 298.15 K in J/kg
  data solid_hf/
    -----1. Kerogen-1 -----      -----2. Kerogen-2 ???-----
    & -1.45d6, 0.0,
    -----3. Kerogen-3 ???-----      -----4. Char-C ??? -----
    & 0.0, 0.0,
    -----5. Char-H ???-----      -----6. Char-O -----
    & 0.0, 0.0,
    -----7. Char-N ???-----      -----8. Char-S -----
    & 0.0, 0.0,
    -----9. Inert -----      -----10. Moisture -----
    & 0.0, -1.588d7,
    -----11. Bound water -----      -----12. CaCO3 -----
    & -1.614d7, -1.2063d7,
    -----13. CaO -----      -----14. CaSO4 -----
    & -1.1325d7, -1.0534d7,
    -----15. MgCO3 -----      -----16. MgO -----
    & -1.2986d7, -1.4925d7,
    -----17. MgSO4 -----      -----18. CaSiO3 -----
    & -1.048d7, -1.362d7,
    -----19. FeS2 -----      -----20. FeS -----
    & -1.4124d6, -1.1485d6,
    -----21. Fe2O3 -----      -----22. SiO2 -----
    & -5.1637d6, -1.518d7,
    -----23. N-inorg ???-----      -----24. Oil-1 -----
    & -0.0, -1.93d6,
    -----25. Oil-2 ???-----      -----26. Oil-3 ??? -----
    & -1.50d6, 0.0,

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c      -----27. Oil-4 ???-----  -----28. Oil-5 ???-----
c      &          0.0,           0.0,
c      -----29. Coke  ???-----  -----30. Char ???-----
c      &          0.0,           0.0,
c      -----31. Solid-A -----  -----32. Solid-B -----
c      &          0.0,           0.0,
c      -----33. Solid-C -----  -----34. Solid-D -----
c      &          0.0,           0.0/
c
c solid heat capacity coefficients a + bT + cT**2 + d*T**-2   J/K/kg
c data solid_cpc/
c      -----1. Kerogen-1 -----  -----2. Kerogen-2 -----
c      & 213.0, 5.22, -1.66d-3, 0.0, 1500.0, 0.0, 0.0, 0.0,
c      -----3. Kerogen-3 -----  -----4. Char-C -----
c      & 1500.0, 0.0, 0.0, 0.0, -267.0, 3.889, -1.845d-3, 0.0,
c      -----5. Char-H -----  -----6. Char-O -----
c      & 4482.0, 17.07, 0.0, 0.0, -267.0, 3.889, -1.845d-3, 0.0,
c      -----7. Char-N -----  -----8. Char-S -----
c      & -267.0, 3.889, -1.845d-3, 0.0, -267.0, 3.889, -1.845d-3, 0.0,
c      -----9. Inert -----  -----10. Moisture -----
c      & 580.8, 1.262, -6.468d-4, -1.27d7, 4184.0, 0.0, 0.0, 0.0,
c      -----11. Bound water -----  -----12. CaCO3 -----
c      & 1680.0, 2.2, 0.0, 0.0, 996.3, 0.269, 0.0, -2.5156d7,
c      -----13. CaO -----  -----14. CaSO4 -----
c      & 882.9, 0.1012, -1.154d-5, -1.431d7, 530.2, 0.715, 0.0, -1.0087d6,
c      ----- 15. MgCO3 (fit to 1000K)
c      & 380.0, 2.029, 8.83d-4, 0.0, 1021.1, 0.433, -1.63d-4, -1.772d7,
c      -----16. MgO -----
c      &
c      -----17. MgSO4 -----
c      & 752.4, 0.630, -1.113d-4, 1.1675d7, 18. CaSiO3 ?? (use SiO2)
c      & 289.0, 1.78, -7.761d-4, 0.0,
c      -----19. FeS2 -----  -----20. FeS -----
c      & 727.3, -0.277, 2.579d-4, -1.326d7, 580.7, 0.1133, 0.0, 0.0,
c      -----21. Fe2O3 -----  -----22. SiO2 -----
c      & -294.2, 2.805, -1.542d-3, 2.285d7, 289.0, 1.78, -7.761d-4, 0.0,
c      -----23. N-inorganic ??----  -----24. Oil-1 -----
c      & -267.0, 3.889, -1.845d-3, 0.0, 1600.0, 0.0, 0.0, 0.0,
c      -----25. Oil-2 ???-----  -----26. Oil-3 ???-----
c      & 1600.0, 0.0, 0.0, 0.0, 1600.0, 0.0, 0.0, 0.0,
c      -----27. Oil-4 ???-----  -----28. Oil-5 -----
c      & 1600.0, 0.0, 0.0, 0.0, 1600.0, 0.0, 0.0, 0.0,
c      -----29. Coke -----  -----30. Char -----
c      & 213.0, 5.22, -1.66d-3, 0.0, 213.0, 5.22, -1.66d-3, 0.0,
c      -----31. Solid-A -----  -----32. Solid-B -----
c      & 1000.0, 0.0, 0.0, 0.0, 1000.0, 0.0, 0.0, 0.0,
c      -----33. Solid-C -----  -----34. Solid-D -----
c      & 1000.0, 0.0, 0.0, 0.0, 1000.0, 0.0, 0.0, 0.0/
c
c liq heat of formation at 298.15 K in J/kg
c (For now use gas values)
c data liq_hf/
c      -----1. Oil-1 ???-----  -----2. Oil-2 ??? -----
c      & -1.74d6,           -1.59d6,
c      -----3. Oil-3 ???-----  -----4. Oil-4 ???-----
c      & -1.56d6,           -1.62d6,
c      -----5. Oil-5 ???-----  -----6. Water -----
c      & -1.62d6,           -1.588d7,
c      -----7. Liquid-A -----  -----8. Liquid-B -----
c      & 0.0,                 0.0 /
c
c liq heat capacity coefficients a + bT + cT**2   J/K/kg
c (For now use gas values)

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c      data liq_cpc/
c          -----1. Oil-1 ???-----
c          & 307.9, 5.10, 1.64d-3,
c          -----3. Oil-3 ???-----
c          & 319.1, 4.99, 1.59d-3,
c          -----5. Oil-5 -----
c          & 316.7, 1.207, 3.835d-4,
c          -----7. Liquid-A -----
c          & 1000.0, 0.0, 0.0,
c          -----2. Oil-2 ???-----
c          317.2, 5.03, 1.63d-3,
c          -----4. Oil-4 -----
c          316.7, 1.207, 3.835d-4,
c          -----6. Water -----
c          4184.0, 0.0, 0.0,
c          -----8. Liquid-B -----
c          1000.0, 0.0, 0.0/
c

c  gas viscosity coefficients a*(T/273)**b   kg/m/s
c      data viscc/
c          -----1. N2 ???-----
c          & 1.73e-5, 0.685,
c          -----3. H2 -----
c          & 8.3e-6, 0.67,
c          -----5. CO2 -----
c          & 1.36e-5, 0.87,
c          -----7. H2S ???-----
c          & 3.6e-5, 0.0,
c          -----9. NH3 ???-----
c          & 3.6e-5, 0.0,
c          -----11. HCN ???-----
c          & 3.6e-5, 0.0,
c          -----13. CH4 -----
c          & 1.6e-5, 0.76,
c          -----15. C2H6 ???-----
c          & 3.6e-5, 0.0,
c          -----17. C3H8 ???-----
c          & 3.6e-5, 0.0,
c          -----19. H12 ???-----
c          & 3.6e-5, 0.0,
c          -----21. Oil-2 ???-----
c          & 3.6e-5, 0.0,
c          -----23. Oil-4 ???-----
c          & 3.6e-5, 0.0,
c          -----25. Gas-A -----
c          & 1.73e-5, 0.685,
c          -----27. Gas-C -----
c          & 1.73e-5, 0.685,
c          -----2. O2 ???-----
c          1.73e-5, 0.685,
c          -----4. CO -----
c          1.69e-5, 0.67,
c          -----6. H2O -----
c          8.8e-6, 1.113,
c          -----8. SO2 ???-----
c          3.6e-5, 0.0,
c          -----10. NO2 ???-----
c          3.6e-5, 0.0,
c          -----12. COS ???-----
c          3.6e-5, 0.0,
c          -----14. C2H4 ???-----
c          3.6e-5, 0.0,
c          -----16. C3H6 ???-----
c          3.6e-5, 0.0,
c          -----18. C5 (1/2*C5H12) ???
c          3.6e-5, 0.0,
c          -----20. Oil-1 ???-----
c          3.6e-5, 0.0,
c          -----22. Oil-3 ???-----
c          3.6e-5, 0.0,
c          -----24. Oil-5 ???-----
c          3.6e-5, 0.0,
c          -----26. Gas-B -----
c          1.73e-5, 0.685,
c          -----28. Gas-D -----
c          1.73e-5, 0.685/
c

c  gas molecular volumes used in Fuller, Scheller & Giddings
c  correlation for gas diffusivities.
c      data gas_mv/
c          -----1. N2 -----
c          & 17.9,
c          -----3. H2 -----
c          & 7.07,
c          -----5. CO2 -----
c          & 26.9,
c          -----7. H2S -----
c          & 21.0,
c          -----9. NH3 -----
c          & 14.9,
c          -----11. HCN -----
c          & 24.2,
c          -----13. CH4 -----
c          & 24.5,
c          -----15. C2H6 -----
c          & 45.0,
c          -----17. C3H8 -----
c          & 65.5,
c          -----19. H12 -----
c          & 24.0,
c          -----2. O2 -----
c          16.6,
c          -----4. CO -----
c          18.9,
c          -----6. H2O -----
c          12.7,
c          -----8. SO2 -----
c          41.1,
c          -----10. NO2 -----
c          16.7,
c          -----12. COS -----
c          39.0,
c          -----14. C2H4 -----
c          41.0,
c          -----16. C3H6 -----
c          61.5,
c          -----18. C5 -----
c          33.0,
c          -----20. Oil-1 -----
c          228.0,

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c      -----21. Oil-2 -----  -----22. Oil-3 -----
c      &      494.0,          664.0,
c      -----23. Oil-4 ???-----  -----24. Oil-5 ???-----
c      &      412.0,          412.0,
c      -----25. Gas-A -----  -----26. Gas-B -----
c      &      17.9,           17.9,
c      -----27. Gas-C -----  -----28. Gas-D -----
c      &      17.9,           17.9/
c
c  gas stoichiometry atoms/molecule
  data gas_c/
c      -----1. N2 -----  -----2. O2 -----
c      &      0.0,           0.0,
c      -----3. H2 -----  -----4. CO -----
c      &      0.0,           1.0,
c      -----5. CO2 -----  -----6. H2O -----
c      &      1.0,           0.0,
c      -----7. H2S -----  -----8. SO2 -----
c      &      0.0,           0.0,
c      -----9. NH3 -----  -----10. NO2 -----
c      &      0.0,           0.0,
c      -----11. HCN -----  -----12. COS -----
c      &      1.0,           1.0,
c      -----13. CH4 -----  -----14. C2H4 -----
c      &      1.0,           2.0,
c      -----15. C2H6 -----  -----16. C3H6 -----
c      &      2.0,           3.0,
c      -----17. C3H8 -----  -----18. C5 -----
c      &      3.0,           5.0,
c      -----19. H12 -----  -----20. Oil-1 -----
c      &      0.0,           11.0,
c      -----21. Oil-2 -----  -----22. Oil-3 -----
c      &      24.0,          32.0,
c      -----23. Oil-4 -----  -----24. Oil-5 -----
c      &      20.0,          20.0,
c      -----25. Gas-A -----  -----26. Gas-B -----
c      &      0.0,           0.0,
c      -----27. Gas-C -----  -----28. Gas-D -----
c      &      0.0,           0.0/
c
c  gas stoichiometry atoms/molecule
  data gas_o/
c      -----1. N2 -----  -----2. O2 -----
c      &      0.0,           2.0,
c      -----3. H2 -----  -----4. CO -----
c      &      0.0,           1.0,
c      -----5. CO2 -----  -----6. H2O -----
c      &      2.0,           1.0,
c      -----7. H2S -----  -----8. SO2 -----
c      &      0.0,           2.0,
c      -----9. NH3 -----  -----10. NO2 -----
c      &      0.0,           2.0,
c      -----11. HCN -----  -----12. COS -----
c      &      0.0,           1.0,
c      -----13. CH4 -----  -----14. C2H4 -----
c      &      0.0,           0.0,
c      -----15. C2H6 -----  -----16. C3H6 -----
c      &      0.0,           0.0,
c      -----17. C3H8 -----  -----18. C5 -----
c      &      0.0,           0.0,
c      -----19. H12 -----  -----20. Oil-1 -----
c      &      0.0,           0.22,
c      -----21. Oil-2 -----  -----22. Oil-3 -----
c      &      0.48,          0.64,
c      -----23. Oil-4 -----  -----24. Oil-5 -----

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&          0.20,
c      -----25. Gas-A ----- 0.20,
&          0.0,
c      -----27. Gas-C ----- 0.0,
&          0.0,
c  gas stoichiometry atoms/molecule
  data gas_h/
c      -----1. N2 ----- 2. O2 -----
&          0.0,          0.0,
c      -----3. H2 ----- 4. CO -----
&          2.0,          0.0,
c      -----5. CO2 ----- 6. H2O -----
&          0.0,          2.0,
c      -----7. H2S ----- 8. SO2 -----
&          2.0,          0.0,
c      -----9. NH3 ----- 10. NO2 -----
&          3.0,          0.0,
c      -----11. HCN ----- 12. COS -----
&          1.0,          0.0,
c      -----13. CH4 ----- 14. C2H4 -----
&          4.0,          4.0,
c      -----15. C2H6 ----- 16. C3H6 -----
&          6.0,          6.0,
c      -----17. C3H8 ----- 18. C5 -----
&          8.0,          0.0,
c      -----19. H12 ----- 20. Oil-1 -----
&          12.0,         17.49,
c      -----21. Oil-2 ----- 22. Oil-3 -----
&          38.16,        50.88,
c      -----23. Oil-4 ----- 24. Oil-5 -----
&          31.2,         31.2,
c      -----25. Gas-A ----- 26. Gas-B -----
&          0.0,          0.0,
c      -----27. Gas-C ----- 28. Gas-D -----
&          0.0,          0.0/
c  gas stoichiometry atoms/molecule
  data gas_n/
c      -----1. N2 ----- 2. O2 -----
&          2.0,          0.0,
c      -----3. H2 ----- 4. CO -----
&          0.0,          0.0,
c      -----5. CO2 ----- 6. H2O -----
&          0.0,          0.0,
c      -----7. H2S ----- 8. SO2 -----
&          0.0,          0.0,
c      -----9. NH3 ----- 10. NO2 -----
&          1.0,          1.0,
c      -----11. HCN ----- 12. COS -----
&          1.0,          0.0,
c      -----13. CH4 ----- 14. C2H4 -----
&          0.0,          0.0,
c      -----15. C2H6 ----- 16. C3H6 -----
&          0.0,          0.0,
c      -----17. C3H8 ----- 18. C5 -----
&          0.0,          0.0,
c      -----19. H12 ----- 20. Oil-1 -----
&          0.0,         0.2629,
c      -----21. Oil-2 ----- 22. Oil-3 -----
&          0.5736,       0.7648,
c      -----23. Oil-4 ----- 24. Oil-5 -----
&          0.38,          0.38,
c      -----25. Gas-A ----- 26. Gas-B -----
&          2.0,          2.0,
c      -----27. Gas-C ----- 28. Gas-D -----

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```

& 2.0,
c 2.0/
c
c gas stoichiometry atoms/molecule
  data gas_s/
c
c   -----1. N2 ----- 2. O2 -----
c   & 0.0, 0.0,
c   -----3. H2 ----- 4. CO -----
c   & 0.0, 0.0,
c   -----5. CO2 ----- 6. H2O -----
c   & 0.0, 0.0,
c   -----7. H2S ----- 8. SO2 -----
c   & 1.0, 1.0,
c   -----9. NH3 ----- 10. NO2 -----
c   & 0.0, 0.0,
c   -----11. HCN ----- 12. COS -----
c   & 0.0, 1.0,
c   -----13. CH4 ----- 14. C2H4 -----
c   & 0.0, 0.0,
c   -----15. C2H6 ----- 16. C3H6 -----
c   & 0.0, 0.0,
c   -----17. C3H8 ----- 18. C5 -----
c   & 0.0, 0.0,
c   -----19. H12 ----- 20. Oil-1 -----
c   & 0.0, 0.0341,
c   -----21. Oil-2 ----- 22. Oil-3 -----
c   & 0.0744, 0.0992,
c   -----23. Oil-4 ----- 24. Oil-5 -----
c   & 0.06, 0.06,
c   -----25. Gas-A ----- 26. Gas-B -----
c   & 0.0, 0.0,
c   -----27. Gas-C ----- 28. Gas-D -----
c   & 0.0, 0.0 /
c
c liq stoichiometry atoms/molecule
  data liq_c/
c
c   -----1. Oil-1 ----- 2. Oil-2 -----
c   & 11.0, 24.0,
c   -----3. Oil-3 ----- 4. Oil-4 -----
c   & 32.0, 20.0,
c   -----5. Oil-5 ----- 6. Water -----
c   & 20.0, 0.0,
c   -----7. Liquid-A ----- 8. Liquid-B -----
c   & 0.0, 0.0 /
c
c liq stoichiometry atoms/molecule
  data liq_h/
c
c   -----1. Oil-1 ----- 2. Oil-2 -----
c   & 17.49, 38.16,
c   -----3. Oil-3 ----- 4. Oil-4 -----
c   & 50.88, 31.2,
c   -----5. Oil-5 ----- 6. Water -----
c   & 31.2, 2.0,
c   -----7. Liquid-A ----- 8. Liquid-B -----
c   & 2.0, 2.0 /
c
c liq stoichiometry atoms/molecule
  data liq_o/
c
c   -----1. Oil-1 ----- 2. Oil-2 -----
c   & 0.22, 0.48,
c   -----3. Oil-3 ----- 4. Oil-4 -----
c   & 0.64, 0.20,
c   -----5. Oil-5 ----- 6. Water -----
c   & 0.20, 1.0,
c   -----7. Liquid-A ----- 8. Liquid-B -----

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```

& 1.0, 1.0 /
c
c liq stoichiometry atoms/molecule
  data liq_n/
c
c   -----1. Oil-1 -----  -----2. Oil-2 -----
c   & 0.2629, 0.5736,
c   -----3. Oil-3 -----  -----4. Oil-4 -----
c   & 0.7648, 0.38,
c   -----5. Oil-5 -----  -----6. Water -----
c   & 0.38, 0.0,
c   -----7. Liquid-A -----  -----8. Liquid-B -----
c   & 0.0, 0.0 /
c
c liq stoichiometry atoms/molecule
  data liq_s/
c
c   -----1. Oil-1 -----  -----2. Oil-2 -----
c   & 0.0341, 0.0744,
c   -----3. Oil-3 -----  -----4. Oil-4 -----
c   & 0.0992, 0.06,
c   -----5. Oil-5 -----  -----6. Water -----
c   & 0.06, 0.0,
c   -----7. Liquid-A -----  -----8. Liquid-B -----
c   & 0.0, 0.0 /
c
c Note for purposes of computing weight fractions of C, H, O, N & S
c the atom weights given at the end of this data statement are used
c along with the osp version of mineall molecular weights.
c For osp weights: Ca=40, Mg=24.3, Fe=55.8, Si 28 amus
c
c           Exact      For osp
c           kg/mol    kg/mol
c   CaCO3 ----- 0.10009  0.100
c   CaO ----- 0.05608  0.056
c   CaSO4 ----- 0.13614  0.136
c   MgCO3 ----- 0.0843
c   MgO ----- 0.04030  0.0403
c   MgSO4 ----- 0.1204   0.1203
c   CaSiO3 ----- 0.116
c   FeS2 ----- 0.11997  0.1198
c   FeS ----- 0.08791  0.0878
c   Fe2O3 ----- 0.1597   0.1596
c   SiO2 ----- 0.060
c
c
c solid composition weight fraction carbon
  data solid_wf_c/ ! all carbons
c
c   -----1. Kerogen-1 -----  -----2. Kerogen-2 ???-----
c   & 0.8374, 1.0,
c   -----3. Kerogen-3 ???-----  -----4. Char-C -----
c   & 1.0, 1.00,
c   -----5. Char-H -----  -----6. Char-O -----
c   & 0.0, 0.0,
c   -----7. Char-N -----  -----8. Char-S -----
c   & 0.0, 0.0,
c   -----9. Inert -----  -----10. Moisture -----
c   & 0.0, 0.0,
c   -----11. Bound water -----  -----12. CaCO3 -----
c   & 0.0, 0.12000,
c   -----13. CaO -----  -----14. CaSO4 -----
c   & 0.0, 0.0,
c   -----15. MgCO3 -----  -----16. MgO -----
c   & 0.14235, 0.0,
c   -----17. MgSO4 -----  -----18. CaSiO3 -----
c   & 0.0, 0.0,
c   -----19. FeS2 -----  -----20. FeS -----

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```

&          0.0,                      0.0,
c   -----21. Fe2O3 -----      -----22. SiO2 -----
&          0.0,                      0.0,
c   -----23. N-inorganic -----  -----24. Oil-1 -----
&          0.0,                      0.8367,
c   -----25. Oil-2 -----      -----26. Oil-3 -----
&          0.8367,                  0.8367,
c   -----27. Oil-4 -----      -----28. Oil-5 -----
&          0.8521,                  0.8521,
c   -----29. Coke ???-----  -----30. Char -----
&          0.9012,                  0.8837,
c   -----31. Solid-A -----  -----32. Solid-B -----
&          0.0,                      0.0,
c   -----33. Solid-C -----  -----34. Solid-D -----
&          0.0,                      0.0/
c

data solid_wf_c_inorg/ ! inorganic carbon (used in inorganic C
c                                balance)
c   -----1. Kerogen-1 -----  -----2. Kerogen-2 -----
&          0.0,                      0.0,
c   -----3. Kerogen-3 -----  -----4. Char-C -----
&          0.0,                      0.0,
c   -----5. Char-H -----  -----6. Char-O -----
&          0.0,                      0.0,
c   -----7. Char-N -----  -----8. Char-S -----
&          0.0,                      0.0,
c   -----9. Inert -----  -----10. Moisture -----
&          0.0,                      0.0,
c   -----11. Bound water -----  -----12. CaCO3 -----
&          0.0,                      0.12000,
c   -----13. CaO -----  -----14. CaSO4 -----
&          0.0,                      0.0,
c   -----15. MgCO3 -----  -----16. MgO -----
&          0.14235,                  0.0,
c   -----17. MgSO4 -----  -----18. CaSiO3 -----
&          0.0,                      0.0,
c   -----19. FeS2 -----  -----20. FeS -----
&          0.0,                      0.0,
c   -----21. Fe2O3 -----  -----22. SiO2 -----
&          0.0,                      0.0,
c   -----23. N-inorganic -----  -----24. Oil-1 -----
&          0.0,                      0.0,
c   -----25. Oil-2 -----  -----26. Oil-3 -----
&          0.0,                      0.0,
c   -----27. Oil-4 -----  -----28. Oil-5 -----
&          0.0,                      0.0,
c   -----29. Coke -----  -----30. Char -----
&          0.0,                      0.0,
c   -----31. Solid-A -----  -----32. Solid-B -----
&          0.0,                      0.0,
c   -----33. Solid-C -----  -----34. Solid-D -----
&          0.0,                      0.0/
c

c solid composition weight fraction hydrogen
  data solid_wf_h/
    -----1. Kerogen-1 -----  -----2. Kerogen-2 ???-----
&          0.1047,                  0.0,
c    -----3. Kerogen-3 ???-----  -----4. Char-C -----
&          0.0,                      0.0,
c    -----5. Char-H -----  -----6. Char-O -----
&          1.0,                      0.0,
c    -----7. Char-N -----  -----8. Char-S -----
&          0.0,                      0.0,
c    -----9. Inert -----  -----10. Moisture -----

```

```

&          0.0,                               0.1111111,
c   -----11. Bound water -----  -----12. CaCO3 -----
&          0.1111111,                           0.0,
c   -----13. CaO -----  -----14. CaSO4 -----
&          0.0,                               0.0,
c   -----15. MgCO3 -----  -----16. MgO -----
&          0.0,                               0.0,
c   -----17. MgSO4 -----  -----18. CaSiO3 -----
&          0.0,                               0.0,
c   -----19. FeS2 -----  -----20. FeS -----
&          0.0,                               0.0,
c   -----21. Fe2O3 -----  -----22. SiO2 -----
&          0.0,                               0.0,
c   -----23. N-inorganic -----  -----24. Oil-1 -----
&          0.0,                               0.1108,
c   -----25. Oil-2 -----  -----26. Oil-3 -----
&          0.1108,                           0.1108,
c   -----27. Oil-4 -----  -----28. Oil-5 -----
&          0.1108,                           0.1108,
c   -----29. Coke ???-----  -----30. Char -----
&          0.0315,                           0.03096,
c   -----31. Solid-A -----  -----32. Solid-B -----
&          0.0,                               0.0,
c   -----33. Solid-C -----  -----34. Solid-D -----
&          0.0,                               0.0/
c

c solid composition weight fraction oxygen
  data solid_wf_o/
    -----1. Kerogen-1 -----  -----2. Kerogen-2 ???-----
&          0.0223,                           0.0,
c   -----3. Kerogen-3 ???-----  -----4. Char-C -----
&          0.0,                               0.0,
c   -----5. Char-H -----  -----6. Char-O -----
&          0.0,                               1.0,
c   -----7. Char-N -----  -----8. Char-S -----
&          0.0,                               0.0,
c   -----9. Inert -----  -----10. Moisture -----
&          0.0,                               0.8999999,
c   -----11. Bound water -----  -----12. CaCO3 -----
&          0.8999999,                           0.48000,
c   -----13. CaO -----  -----14. CaSO4 -----
&          0.28571,                           0.47059,
c   -----15. MgCO3 -----  -----16. MgO -----
&          0.56940,                           0.39702,
c   -----17. MgSO4 -----  -----18. CaSiO3 -----
&          0.53200,                           0.4138,
c   -----19. FeS2 -----  -----20. FeS -----
&          0.0,                               0.0,
c   -----21. Fe2O3 -----  -----22. SiO2 -----
&          0.30075,                           0.533333,
c   -----23. N-inorganic -----  -----24. Oil-1 -----
&          0.0,                               0.0223,
c   -----25. Oil-2 -----  -----26. Oil-3 -----
&          0.0223,                           0.0223,
c   -----27. Oil-4 -----  -----28. Oil-5 -----
&          0.0114,                           0.0114,
c   -----29. Coke -----  -----30. Char -----
&          0.0240,                           0.02334,
c   -----31. Solid-A -----  -----32. Solid-B -----
&          0.0,                               0.0,
c   -----33. Solid-C -----  -----34. Solid-D -----
&          0.0,                               0.0/
c

c solid composition weight fraction nitrogen

```

```

c      data solid_wf_n/
c          -----1. Kerogen-1 -----  -----2. Kerogen-2 ????-----
c          &           0.0244,           0.0,
c          -----3. Kerogen-3 ???-----  -----4. Char-C -----
c          &           0.0,           0.0,
c          -----5. Char-H -----  -----6. Char-O -----
c          &           0.0,           0.0,
c          -----7. Char-N -----  -----8. Char-S -----
c          &           1.0,           0.0,
c          -----9. Inert -----  -----10. Moisture -----
c          &           0.0,           0.0,
c          -----11. Bound water -----  -----12. CaCO3 -----
c          &           0.0,           0.0,
c          -----13. CaO -----  -----14. CaSO4 -----
c          &           0.0,           0.0,
c          -----15. MgCO3 -----  -----16. MgO -----
c          &           0.0,           0.0,
c          -----17. MgSO4 -----  -----18. CaSiO3 -----
c          &           0.0,           0.0,
c          -----19. FeS2 -----  -----20. FeS -----
c          &           0.0,           0.0,
c          -----21. Fe2O3 -----  -----22. SiO2 -----
c          &           0.0,           0.0,
c          -----23. N-inorganic -----  -----24. Oil-1 -----
c          &           0.0,           0.0233,
c          -----25. Oil-2 -----  -----26. Oil-3 -----
c          &           0.0233,           0.0233,
c          -----27. Oil-4 -----  -----28. Oil-5 -----
c          &           0.0189,           0.0189,
c          -----29. Coke ???-----  -----30. Char -----
c          &           0.0336,           0.0430,
c          -----31. Solid-A -----  -----32. Solid-B -----
c          &           0.0,           0.0,
c          -----33. Solid-C -----  -----34. Solid-D -----
c          &           0.0,           0.0/
c
c solid composition weight fraction sulfur
  data solid_wf_s/
    -----1. Kerogen-1 -----  -----2. Kerogen-2 ????-----
    &           0.0112,           0.0,
    -----3. Kerogen-3 ???-----  -----4. Char-C -----
    &           0.0,           0.0,
    -----5. Char-H -----  -----6. Char-O -----
    &           0.0,           0.0,
    -----7. Char-N -----  -----8. Char-S -----
    &           0.0,           1.0,
    -----9. Inert -----  -----10. Moisture -----
    &           0.0,           0.0,
    -----11. Bound water -----  -----12. CaCO3 -----
    &           0.0,           0.0,
    -----13. CaO -----  -----14. CaSO4 -----
    &           0.0,           0.235294,
    -----15. MgCO3 -----  -----16. MgO -----
    &           0.0,           0.0,
    -----17. MgSO4 -----  -----18. CaSiO3 -----
    &           0.266002,           0.0,
    -----19. FeS2 -----  -----20. FeS -----
    &           0.53422,           0.36445,
    -----21. Fe2O3 -----  -----22. SiO2 -----
    &           0.0,           0.0,
    -----23. N-inorganic -----  -----24. Oil-1 -----
    &           0.0,           0.0069,
    -----25. Oil-2 -----  -----26. Oil-3 -----
    &           0.0069,           0.0069,

```

```

c      -----27. Oil-4 -----      -----28. Oil-5 -----
c      &          0.0068,           0.0068,
c      -----29. Coke -----      -----30. Char -----
c      &          0.0096,           0.01904,
c      -----31. Solid-A -----      -----32. Solid-B -----
c      &          0.0,               0.0,
c      -----33. Solid-C -----      -----34. Solid-D -----
c      &          0.0,               0.0/
c
c solid densities (kg/m**3)
  data solid_rho/
    -----1. Kerogen-1 -----      -----2. Kerogen-2 ???-----
    &          1050.0,            1000.0,
    -----3. Kerogen-3 ???-----      -----4. Char-C ???-----
    &          1000.0,            1050.0,
    -----5. Char-H ???-----      -----6. Char-O ???-----
    &          1050.0,            1050.0,
    -----7. Char-N ???-----      -----8. Char-S ???-----
    &          1050.0,            1050.0,
    -----9. Inert -----      -----10. Moisture ???-----
    &          2650.0,            1000.0,
    -----11. Bound water ???---      -----12. CaCO3 -----
    &          1000.0,            2710.0,
    -----13. CaO -----      -----14. CaSO4 -----
    &          3350.0,            2960.0,
    -----15. MgCO3 ???-----      -----16. MgO -----
    &          2850.0,            3580.0,
    -----17. MgSO4 ???-----      -----18. CaSiO3 ???????
    &          2650.0,            2650.0,
    -----19. FeS2 -----      -----20. FeS -----
    &          4980.0,            4830.0,
    -----21. Fe2O3 -----      -----22. SiO2 -----
    &          5280.0,            2650.0,
    -----23. N-inorganic ???---      -----24. Oil-1 ???-----
    &          2650.0,            1050.0,
    -----25. Oil-2 ???-----      -----26. Oil-3 ???-----
    &          1050.0,            1050.0,
    -----27. Oil-4 ???-----      -----28. Oil-5 ???-----
    &          1050.0,            1050.0,
    -----29. Coke ???-----      -----30. Char -----
    &          1050.0,            1050.0,
    -----31. Solid-A -----      -----32. Solid-B -----
    &          2000.0,            2000.0,
    -----33. Solid-C -----      -----34. Solid-D -----
    &          2000.0,            2000.0/
c
c define elemental molecular weights in kg/mol units
  data mw_c/0.012/, mw_h/0.001/, mw_o/0.016/, mw_n/0.014/,
&      mw_s/0.032/

```

Reaction names from reaction.f routine associated with rate_setup_stoich.

```

  data reaction_name/
& 'KER-1 + O2 ', 'KER-2 + O2 ', 'KER-3 + O2 ', ! 1 2 3
& 'CHAR-C + O2 ', 'CHAR-H + O2 ', 'CHAR-O + O2 ', ! 4 5 6
& 'CHAR-N + O2 ', 'CHAR-S + O2 ', 'MGC03 DECOMP', ! 7 8 9
& 'CACO3 DECOMP', 'KER-1 P L ', 'KER-1 P G ', ! 10 11 12
& 'OIL-1 ADS ', 'OIL-2 ADS ', 'OIL-3 ADS ', ! 13 14 15
& 'OIL-1 COK ', 'OIL-2 COK ', 'OIL-3 COK ', ! 16 17 18
& 'COKE + O2 ', 'OIL-1 EVAP ', 'OIL-2 EVAP ', ! 19 20 21
& 'OIL-3 EVAP ', 'CHAR + O2 ', 'FES2 COMB ', ! 22 23 24

```

```

& 'CACO3 + SIO2', 'EXTRA 1      ', 'EXTRA 2      ', ! 25 26 27
& 'EXTRA 3      ', 'EXTRA 4      '/                  ! 28 29

*****
Stoichiometric defaults from reaction.f routine rate_setup_stoich.
*****



c
c 1. kerogen-1 + o2
  call combust((solid_wf_c(1)),(solid_wf_h(1)),(solid_wf_o(1)),
  &           (solid_wf_n(1)),(solid_wf_s(1)),
  &           ao2,aco2,ah2o,ano2,aso2)
  s_stoich(1,1)=-1.0
  g_stoich(2,1)=-ao2
  g_stoich(5,1)=aco2
  g_stoich(6,1)=ah2o
  g_stoich(8,1)=aso2
  g_stoich(10,1)=ano2
c
c 2. kerogen-2 + o2
  call combust((solid_wf_c(2)),(solid_wf_h(2)),(solid_wf_o(2)),
  &           (solid_wf_n(2)),(solid_wf_s(2)),
  &           ao2,aco2,ah2o,ano2,aso2)
  s_stoich(2,2)=-1.0
  g_stoich(2,2)=-ao2
  g_stoich(5,2)=aco2
  g_stoich(6,2)=ah2o
  g_stoich(8,2)=aso2
  g_stoich(10,2)=ano2
c
c 3. kerogen-3 + o2
  call combust((solid_wf_c(3)),(solid_wf_h(3)),(solid_wf_o(3)),
  &           (solid_wf_n(3)),(solid_wf_s(3)),
  &           ao2,aco2,ah2o,ano2,aso2)
  s_stoich(3,3)=-1.0
  g_stoich(2,3)=-ao2
  g_stoich(5,3)=aco2
  g_stoich(6,3)=ah2o
  g_stoich(8,3)=aso2
  g_stoich(10,3)=ano2
c
c 4. char-C + O2
  s_stoich(4,4)=-1.0
  g_stoich(2,4)=-1.0/mw_c
  g_stoich(5,4)=1.0/mw_c
c
c 5. char-H + O2
  s_stoich(5,5)=-1.0
  g_stoich(2,5)=-1.0/mw_h/4.0
  g_stoich(6,5)=1.0/mw_h/2.0
c
c 6. char-O + O2
  s_stoich(6,6)=-1.0
  g_stoich(2,6)=1.0/mw_o/2.0
c
c 7. char-N + O2
  s_stoich(7,7)=-1.0
  g_stoich(2,7)=-1.0/mw_n
  g_stoich(10,7)=1.0/mw_n
c
c 8. char-S + O2
  s_stoich(8,8)=-1.0
  g_stoich(2,8)=-1.0/mw_s
  g_stoich(8,8)=1.0/mw_s

```

```

c
c 9. MgCO3 decomposition
  s_stoich(15,9)=-1.0
  s_stoich(16,9)=0.478055
  g_stoich( 5,9)=11.8624
c
c 10. CaCO3 decomposition
  s_stoich(12,10)=-1.0
  s_stoich(13,10)=0.560008
  g_stoich( 5,10)=10.000
c
c 11. Kerogen-1 decomposition (basis per kg kerogen) to liquid oil
  s_stoich( 1,11)=-1.0          ! Kerogen
  s_stoich(30,11)=0.16280        ! Char
  g_stoich( 3,11)=1.65909        ! H2
  g_stoich( 6,11)=0.118345       ! H2O
  g_stoich( 7,11)=0.092250       ! H2S
  g_stoich( 9,11)=0.00256086     ! NH3
  g_stoich(13,11)=0.8000         ! CH4
  g_stoich(14,11)=0.5600         ! C2H4
  g_stoich(16,11)=1.32659        ! C3H6
  l_stoich( 1,11)=0.372187
  l_stoich( 2,11)=0.186094
  l_stoich( 3,11)=0.186094
c
c 12. Kerogen-1 decomposition (basis per kg kerogen) to gas phase oil
  call move(s_stoich(1,11),s_stoich(1,12),ncomp_solid)
  call move(g_stoich(1,11),g_stoich(1,12),ncomp_gas)
  g_stoich(20,12)=l_stoich(1,11)/gas_mw(20)
  g_stoich(21,12)=l_stoich(2,11)/gas_mw(21)
  g_stoich(22,12)=l_stoich(3,11)/gas_mw(22)
c
c 13. Oil-1(g) > oil-1(s) (basis one mole of gas)
  g_stoich(20,13)=-1.0
  s_stoich(24,13)= gas_mw(20)
c
c 14. Oil-2(g) > oil-2(s) (basis one mole of gas)
  g_stoich(21,14)=-1.0
  s_stoich(25,14)= gas_mw(21)
c
c 15. Oil-1(g) > oil-1(s) (basis one mole of gas)
  g_stoich(22,15)=-1.0
  s_stoich(26,15)= gas_mw(22)
c
c 16. Oil-1(s) > coke + gases
  s_stoich(24,16)=-1.0          ! Oil
  s_stoich(29,16)=0.68           ! Coke
  g_stoich( 3,16)=21.0332         ! H2
  g_stoich( 5,16)=0.141875        ! CO2
  g_stoich( 6,16)=0.0900           ! H2O
  g_stoich( 7,16)=0.011625         ! H2S
  g_stoich( 9,16)=0.0322857       ! NH3
  g_stoich(13,16)=5.0             ! CH4
  g_stoich(14,16)=3.5             ! C2H4
  g_stoich(16,16)=2.16893          ! C3H6
c
c 17. Oil-2(s) > coke + gases
  s_stoich(25,17)=-1.0          ! Oil
  s_stoich(29,17)=0.68           ! Coke
  g_stoich( 3,17)=21.0332         ! H2
  g_stoich( 5,17)=0.141875        ! CO2
  g_stoich( 6,17)=0.0900           ! H2O
  g_stoich( 7,17)=0.011625         ! H2S
  g_stoich( 9,17)=0.0322857       ! NH3

```

```

g_stoich(13,17)=5.0          ! CH4
g_stoich(14,17)=3.5          ! C2H4
g_stoich(16,17)=2.16893      ! C3H6
c
c 18. oil-2(s) > coke + gases
s_stoich(26,18)=-1.0         ! Oil
s_stoich(29,18)=0.68          ! Coke
g_stoich( 3,18)=21.0332       ! H2
g_stoich( 5,18)=0.141875      ! CO2
g_stoich( 6,18)=0.0900        ! H2O
g_stoich( 7,18)=0.011625      ! H2S
g_stoich( 9,18)=0.0322857     ! NH3
g_stoich(13,18)=5.0          ! CH4
g_stoich(14,18)=3.5          ! C2H4
g_stoich(16,18)=2.16893      ! C3H6
c
c 19. Coke + o2
call combust((solid_wf_c(29)),(solid_wf_h(29)),
&           (solid_wf_o(29)),(solid_wf_n(29)),
&           (solid_wf_s(29)),
&           ao2,aco2,ah2o,ano2,aso2)
s_stoich(29,19)=-1.0
g_stoich(2,19)=-ao2
g_stoich(5,19)=aco2
g_stoich(6,19)=ah2o
g_stoich(8,19)=aso2
g_stoich(10,19)=ano2
c
c 20. Evap of liq Oil-1 to gas Oil-1
l_stoich( 1,20) = -1.0
g_stoich(20,20) = -l_stoich(1,20)/gas_mw(20)
c
c 21. Evap of liq Oil-2 to gas Oil-2
l_stoich( 2,21) = -1.0
g_stoich(21,21) = -l_stoich(2,21)/gas_mw(21)
c
c 22. Evap of liq Oil-3 to gas Oil-3
l_stoich( 3,22) = -1.0
g_stoich(22,22) = -l_stoich(3,22)/gas_mw(22)
c
c 23. Composite Char + O2 > combustion products
call combust((solid_wf_c(30)),(solid_wf_h(30)),(solid_wf_o(30)),
&           (solid_wf_n(30)),(solid_wf_s(30)),
&           ao2,aco2,ah2o,ano2,aso2)
s_stoich(30,23)=-1.0
g_stoich( 2,23)=-ao2
g_stoich( 5,23)=aco2
g_stoich( 6,23)=ah2o
g_stoich( 8,23)=aso2
g_stoich(10,23)=ano2
c
c 24. Net Combustion of FeS2
FeS2 + 2CaCO3 + 3.75O2 > 0.5Fe2O3 + 2CaSO4 + 2CO2
s_stoich(19,24)=-1.0
s_stoich(12,24)=-1.66945
s_stoich(21,24)= 0.666128
s_stoich(14,24)= 2.27044
g_stoich( 2,24)=-31.3022
g_stoich( 5,24)= 16.6945
c
c 25. CaCO3 + SiO2 > CaSiO3 + CO2
s_stoich(12,25)=-1.0
s_stoich(22,25)=-0.6
s_stoich(18,25)= 1.16

```

```
g_stoich( 5,25)=10.000
c
c 26. Extra 1. No defined stoich or kinetics
c
c 27. Extra 2. No defined stoich or kinetics
c
c 28. Extra 3. No defined stoich or kinetics
c
c 29. Extra 4. No defined stoich or kinetics
```

APPENDIX B

EXAMPLE: NINE PARTICLE RETORT SIMULATION

The following describes an OSP run in which LLNL's 4TU-Pilot is simulated by the OSP model. The 4TU-Pilot retort uses a Hot-Recycled-Solids process. In the unit shown schematically in Figure B1, processing begins as raw feed and recycled shale are mixed in a fluidized bed (FBM), at a ratio of approximately 1:3. This compact unit rapidly mixes the two streams with a 30 second average solids residence time. The combined stream leaving the mixer is in thermal equilibrium at retorting temperature (approx. 500°C), next spends 2-3 minutes in a gravity flow pyrolyzer (PYR), where complete pyrolysis takes place. This moving packed bed has the advantage of uniform solid residence time and the ability to hold and process fines, which would be rejected from a fluidized bed pyrolyzer. The pyrolyzer also serves as a surge tank with excess capacity to accommodate temporary process upsets. The condensable oil and gas, containing water and dust, pass through staged coolers for product recovery. After cooling, the non condensable gas is either discharged or recycled back to fluidize the mixer. The solid leaving the pyrolyzer enters the pneumatic lift-pipe (LFT), where residual carbon on the spent shale is combusted during transport to the top of the tower. The lift discharges into a delayed-fall combustor (DFC), which provides an additional 5 second residence time for shale combustion in a compact 2.5 meter unit. Below the DFC, the gas and solid is separated with the solid entering a fluid-bed classifier (FBC). This unit has two functions. First, it classifies the shale, discharging the smaller material into the spent shale hopper and recycling the larger shale back to the fluid-bed mixer. Second, it provides a pressure block to balance the loop, keeping separate the combustion and pyrolysis atmospheres of the process.

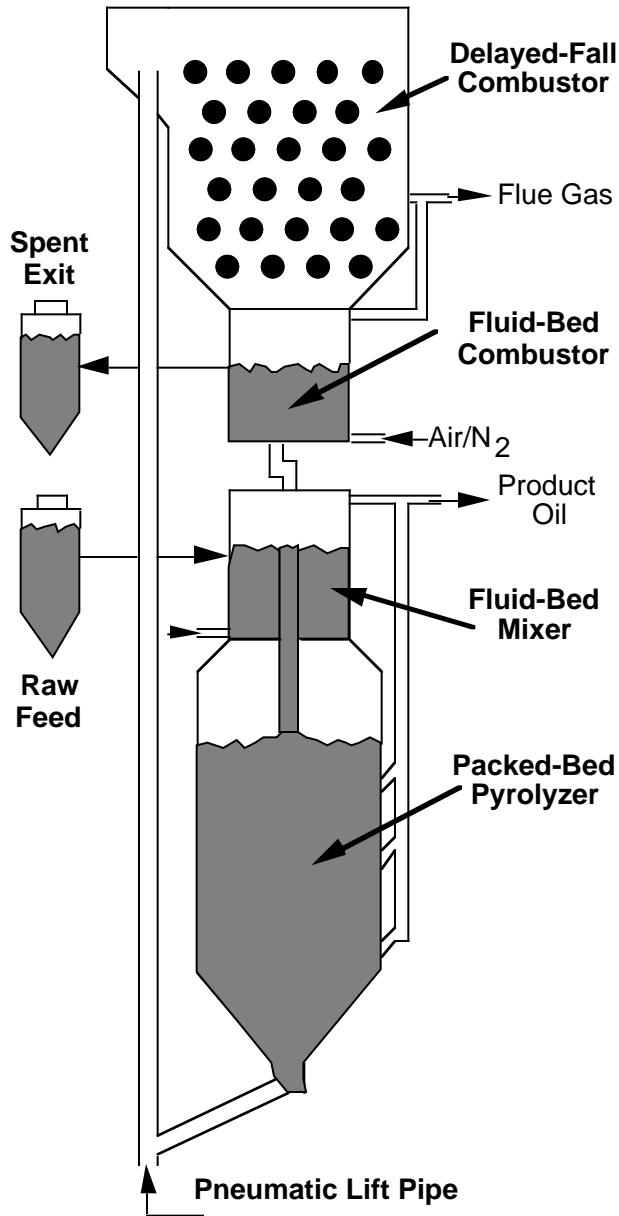


Figure B1. Schematic of the 4TU-Pilot Retort.

In simulating the 4TU-Pilot with OSP, computational modules are logically broken into ten process areas. These areas and the overall flow of process streams is shown in Figure B2. The labels on the arrows into and out of the system are names of process streams entering and leaving the system. In these names, as in those used for the rest of the streams, the notation "A-D" means that the name is repeated once for each letter between "A" and "D". These letters are used to identify the size class of solid streams.

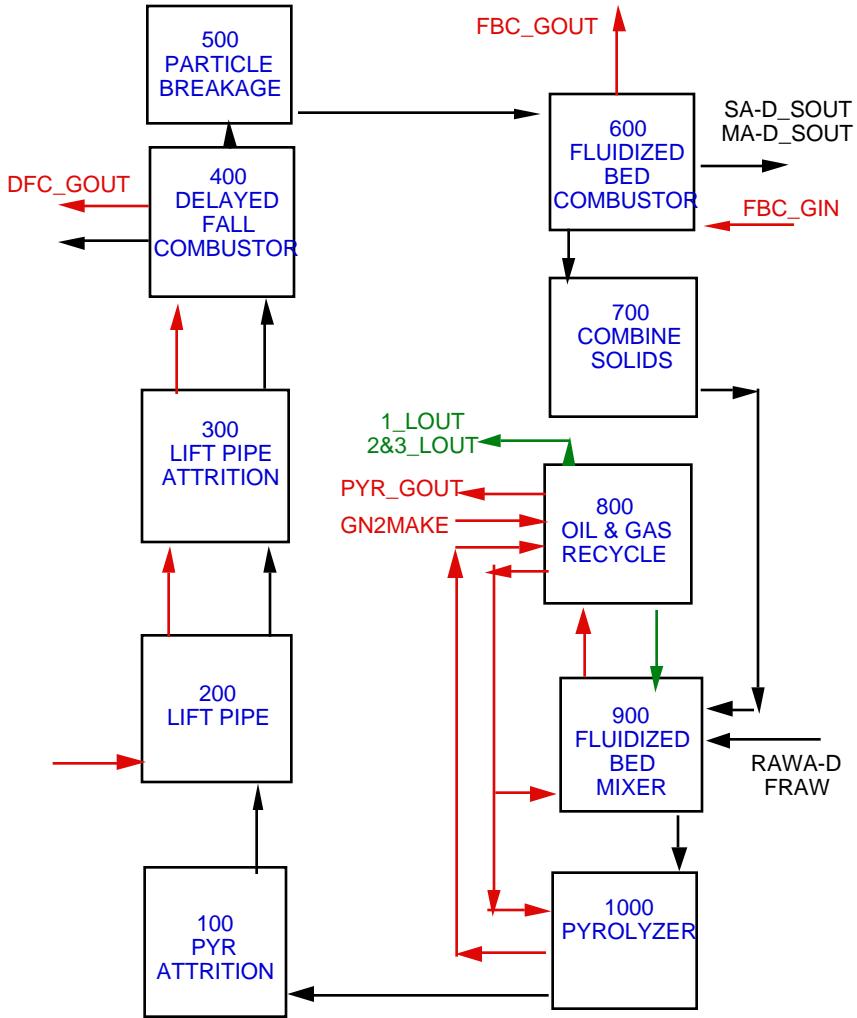


Figure B2. OSP Plant Areas with Input & Output Streams Labeled.

In developing the input for the simulation, several naming conventions have been used. First, all streams which flow between one process module and another are given primarily numeric names. The numeric part of the name is derived from the unit from which the stream exits. Additionally, gas streams begin with the letter "G" and liquid streams with the letter "L". Solid streams begin with the letter "S" if the stream represents single pass solid (i.e. solid going around the process loop for the first time). The letter "M" is used to designate multi-pass solid streams and the letter "F" is reserved for solid streams composed of fines.

Streams which exit or enter the overall process are given primarily non-numeric names. This distinguishes them from connecting streams and is useful in insuring the streams are properly connected since OSP lists for the user those streams which have been called out by computational modules an odd number of times. If the above naming convention has been followed all the names in this list should be predominately non-numeric, any predominately numeric names probably indicate an error has been made in specifying input information.

INPUT FILE DESCRIPTION

The complete input file is listed at the end of this appendix. Those lines beginning with a "*" are comment lines. Also, comments are sometimes included on data lines. In particular note is often made of the units. It should be remembered that these comments have no effect on execution of the code, noting an input in a different unit set than called for does not make the input correct.

In the following discussion frequent reference will be made to this input file. \$GLOBAL, \$PROPERTY and \$FLAG areas will first be described, followed by a discussion of input required for each of the 10 plant areas and finally stream initializations. In this discussion, as in the body of the report, variables are referred to using capital letters in the text. This is done to reduce confusion in the text. However, note that there is essentially no case sensitivity to the OSP input (the exception is ASCII title and description strings) and in general lower case has been used in the input file.

The \$GLOBAL section includes only two lines of data input. A maximum of 31 loops to reach a converged solution will be allowed and the error criteria for each module must be less than 2×10^{-4} for a solution to be considered converged. These errors are generally temperature measures and this tolerance represents a few tenths of a degree. Multiple passes through the computation modules is required for this simulation because of the presence of recycle streams. Also defined is one internal computation group which is to be repeated twice for each overall pass. The members of this group will be noted in the discussion of the computational modules.

The page or two of comments in the input file following the \$GLOBAL section has been generated to allow this file to be more easily used as a template for other simulations of the 4TU-Pilot. The comments document those locations where changes in input values would most likely be required for a simulation of a different pilot experiment.

The \$PROPERTIES input section consists of only eight non comment lines. This means that many of the default property values are in use for this simulation.

In the next section of the input file starting at the line "* Set global flags ...", species and reaction flags are set which will later be used by the main reaction modules. Flags have been set for the combustion side of the process and the pyrolysis side. In addition, a set labeled "COMB-FBC" is included since in some simulations there is no oxygen injection into the FBC. In this case the modules simulating the FBC run more rapidly and smoothly if the combustion reactions are explicitly turned off. In addition the kerogen content in this group is omitted from the solid species list since all residual kerogen is consumed in the LFT and DFC.

The next several pages of the input file define the computational modules, their parameters and the stream connections. Note that the order in which the modules will be executed is given by the order in which they appear. Each module has been given a descriptive name and

a unique tag number. The tag number is derived from the plant area in which the module is located.

The exit of the pyrolyzer has been chosen as the point to begin the computations. This was selected because it is possible to make reasonable guesses about the composition and temperature of the solid streams at this point. The ability to make reasonable guesses is of limited usefulness in causing a solution to converge rapidly, unless the guesses are very good. This is because a tight tolerance is generally enforced on the final iterated solution and the convergence is at best linear since a simple functional iteration approach is used. It is more important to make reasonable guesses to insure that the solution that is finally produced by the simulation is the one intended. Since the system is nonlinear, there is potentially more than a single solution to the system. In general, most of the solutions are non physical, negative compositions or temperatures, and will not be found by OSP because of checks put into various computational modules. However, in some cases there are more than one physically realistic solution and the one that is reached is dependent on the starting guess.

Plant Area 100

The first module defined is a simple PASS_THRU module. It has been made part of plant area 100. Figure B3 is a schematic of the 100 area module connections. The RELAX module is used to isolate one computational loops results from the next. If it was not present then when the final solution is reached, the reaction module computing the exit streams from the PYR would overwrite the stream values used at the start of the final loop. Particularly for debugging purposes, this is undesirable. This sort of stream overwrite occurs in other parts of the system due to internal recycle streams. In general no attempt has been made to remove all the overwrite situations. However, if difficulty develops with a solution the user may want to add PASS_THRU modules in all recycle loops to help reduce the confusion about operation of individual modules. In regard to tracking down computational difficulties, the user should make use of the restart capabilities and the ability to make modified input files which will help determine the root of the problems.

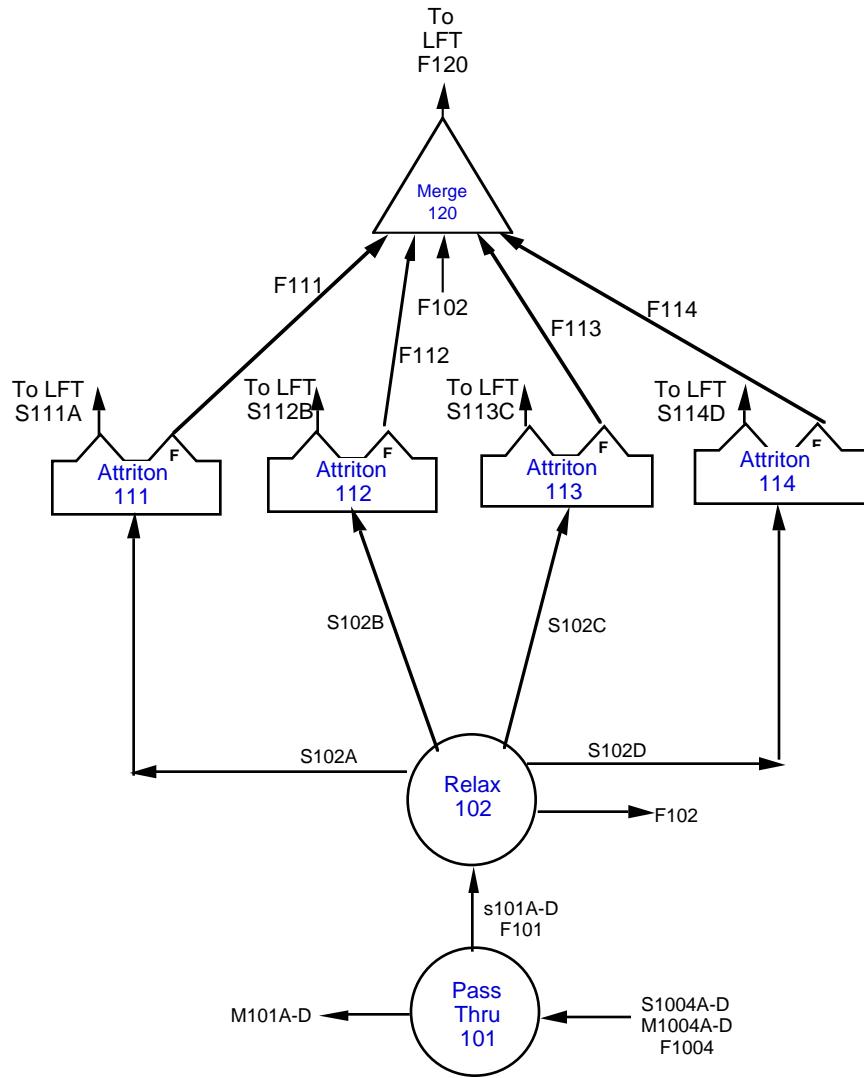


Figure B3. Plant Area 100 - PYR Attrition.

The next group of modules forms the Pyrolyzer Attrition Train which forms the bulk of plant area 100. The first module in this train is a RELAX module (tag=102). This has been included so that relaxation of solid compositions can be invoked if instability develops in the overall iteration scheme. The RELAX parameter is set to one in this example which means the relaxation feature is not active. Solution of this system does require relaxation. A relatively smooth iteration to a converged solution occurs for all values of input streams variables used to date.

The next four modules are ATTRITION modules which are used to generate fines from a specified fraction of each size class of single-pass material. This section ends with a MERGE_STRM module used to collect all the fines streams into a single stream to be sent to the LFT.

Plant Area 200

The next section describes the Lift Pipe Train and is plant area 200, shown schematically in Figure B4. It is composed of a single LIFT_PIPE module which performs the calculations for the LFT unit. In this module the DEL_COKE_COMB parameter has been redefined from its default value of 0.105 to 0.02 to increase the speed of coke combustion. The module uses the COMB flags for species and reactions.

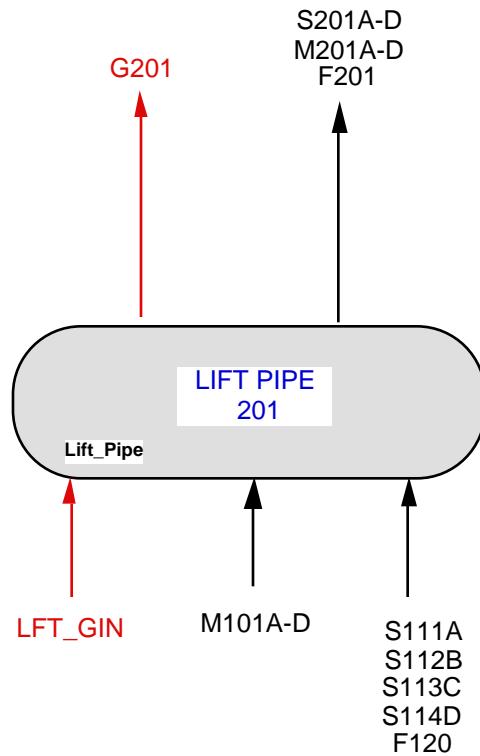


Figure B4. Plant Area 200 - LFT.

Plant Area 300

Plant area 300 modules follow (Figure B5). These modules are used to describe the attrition of particles after they exit the LFT. Eight ATTRITION modules are used to describe attrition of both single and multiple pass particles. In this case attrition TYPE=2 is used to model the attrition of the outer ash layer. Two MERGE_STRMS modules complete the 300 area and are used to collect all the fines streams together into a single stream to be passed on to the DFC.

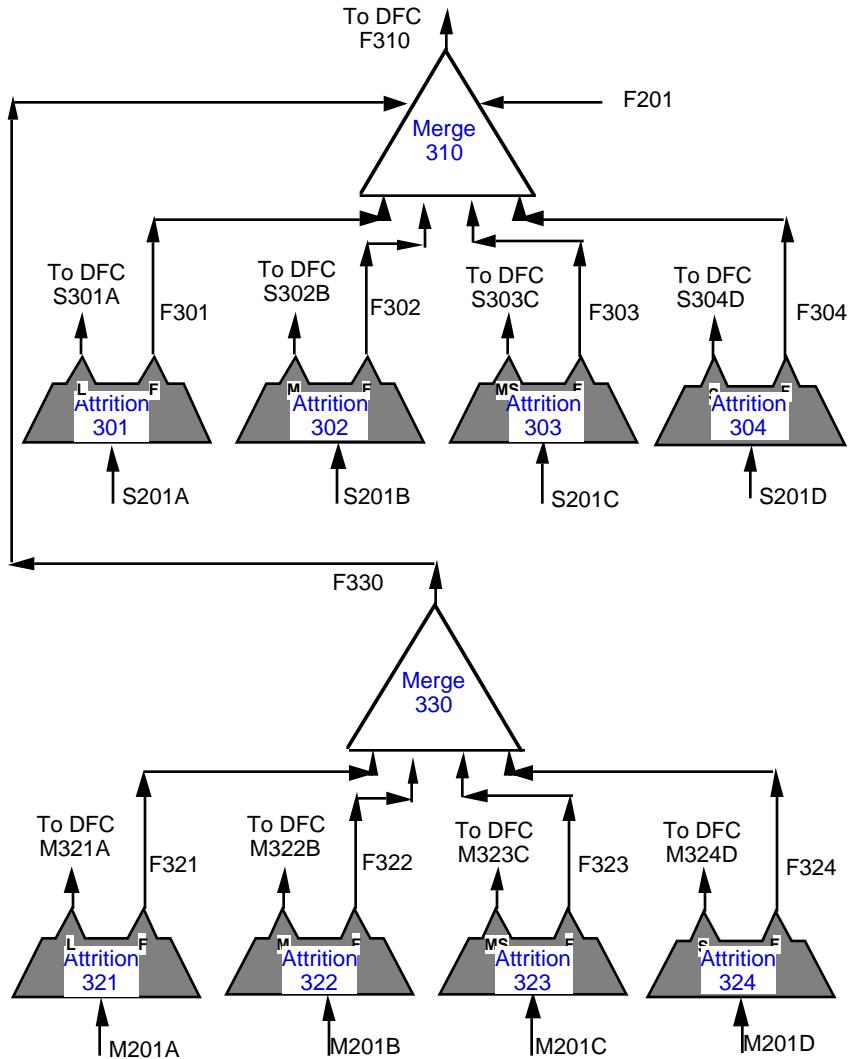


Figure B5. Plant Area 300 - LFT Attrition.

Plant Area 400

Plant area 400, Figure B6, is next. It is made up of two computational modules. The first is a CO_CURRENT module which is used to model the main DFC unit. Again, COMB reaction and species flags are used to describe interaction between seven solid streams and the gas stream. The IDILUTE and IBED parameters are set to use dilute phase correlations. This is not strictly necessary since the values used are also the default values. The second module is a LIFT_PIPE module which is used to model the annular space in the DFC unit through which the gas & fines exit the system. Rather than compute the solid velocity a small slip velocity is set and the fines travel through at approximately the gas velocity. The streams leaving the module exit the system and therefore have been given non-numeric names.

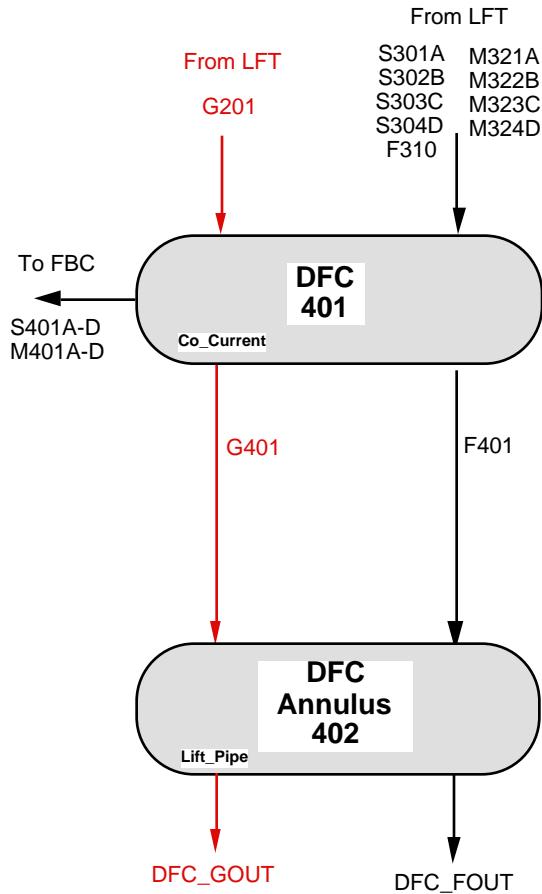


Figure B6. Plant Area 400 - DFC.

Plant Area 500

The next plant area, 500 (Figure B7), describes the breakage of particles after they have passed through the DFC. In this case, as with other modules which modify the particle distribution, the lumping of all changes into discrete locations is only an approximation of the true physical processes. A series of TYPE=1 ATTRITION modules are used to describe the breaking of the top three size classes for both single and multiple pass solids into smaller particle size classes. A series of MERGE_STRMS modules are used to combine all particles of the same size class and type (single or multiple pass) so that emerging from this plant area are eight solid streams, four size classes for each type. The breakage model used here deals with only non-fines. The streams exiting this plant area pass onto the FBC unit.

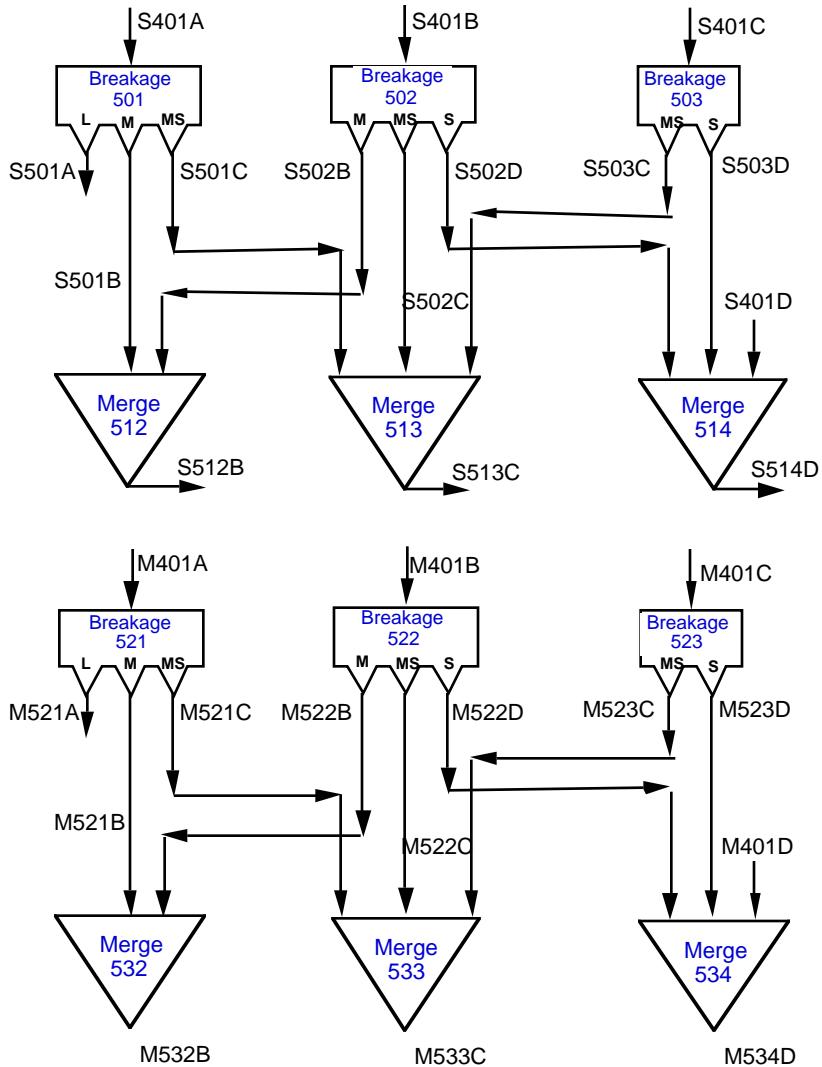


Figure B7. Plant Area 500 - Particle Breakage.

Plant Area 600

In the next plant area, 600 (Figure B8), are modules to simulate the FBC. Two main reaction modules are used to describe the FBC. Both are CSTR modules used to simulate simple fluidized beds. In each module a particle size distribution has been input. This distribution groups single and multiple pass particles in the same size categories together in establishing the distribution within the units. The same distribution is used in both CSTR modules. The FBC bed has been, somewhat arbitrarily, broken into two parts representing the upper one third of the bed and the lower two thirds. Between these modules are a series of four SPLIT_STRMS modules which are used to control the recycle rate of solids. It is assumed that classification occurs in the bed, but single and multiple pass particles belonging to the same size class behave identically. Consequently, each SPLIT_STRMS module has two solid streams entering and exiting. The same fraction of each stream is taken to make the required flow exiting the system. Again, non numeric names are given to those streams exiting the system.

All the modules in this plant area have been included in GROUP 1. This set forms an internal iteration loop. This was done because of the counter current nature (i.e. the gas flows counter to the direction of the sweep of calculations) of the gas stream. Because of this, a MERGE_STRMS module has been used to provide a measure of convergence for this inner loop. Modules in this group are executed twice (dictated by the setting in \$GLOBAL of GROUP_LOOP(1) parameter to 2) for each overall iteration.

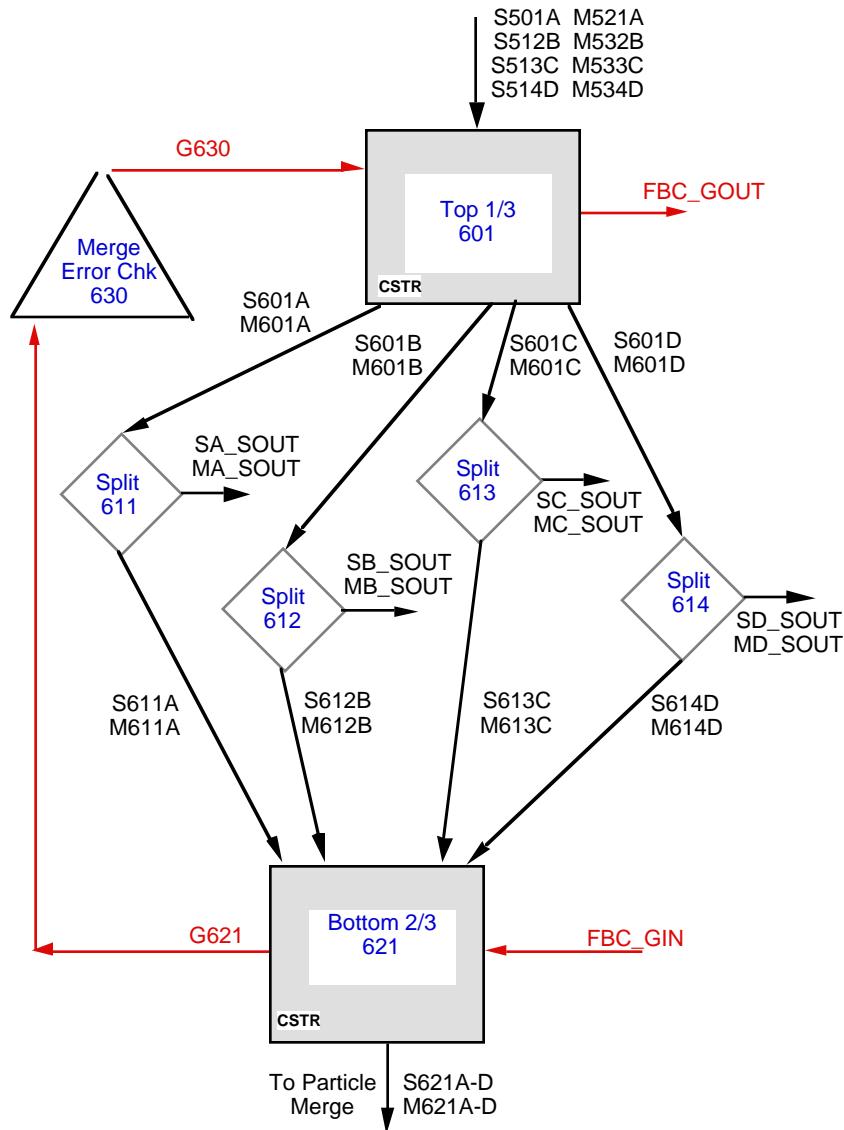


Figure B8. Plant Area 600 - FBC.

Plant Area 700

Figure B9 shows plant area 700 where single and multiple pass streams are merged to make the recycle, or multiple pass, streams to be sent on to the FBC. This is accomplished using four MERGE_STRMS modules. Also entering and leaving each module is a gas cooling stream. This is not part of the physical process but is included to allow for a greater control over the

simulation. The flow rate of the gas cooling stream is taken to be a very large value and thus its temperature effectively is used to set the temperature of the recycled solids. This temperature is varied until a match is obtained between measured and computed temperatures in the PYR. The relative amount of heating or cooling can be obtained through the use of auxiliary modules. They could be included in this simulation file, however, they and other modules used to obtain overall operation summaries are included in a second input file run after the completion of the main simulation. (This file and its uses are outlined in the example in Appendix B.) Notice that the same gas streams are used by each of the four MERGE_STRMS modules. If this was a real process stream this would not make any sense. However, in this case using the same stream over reduces the number of input streams which have to be initialized. The user should be aware that multiple uses of even true process streams are often useful. In one case they can be used in the actual process module which simulates the desired operation and then used again to obtain some auxiliary information.

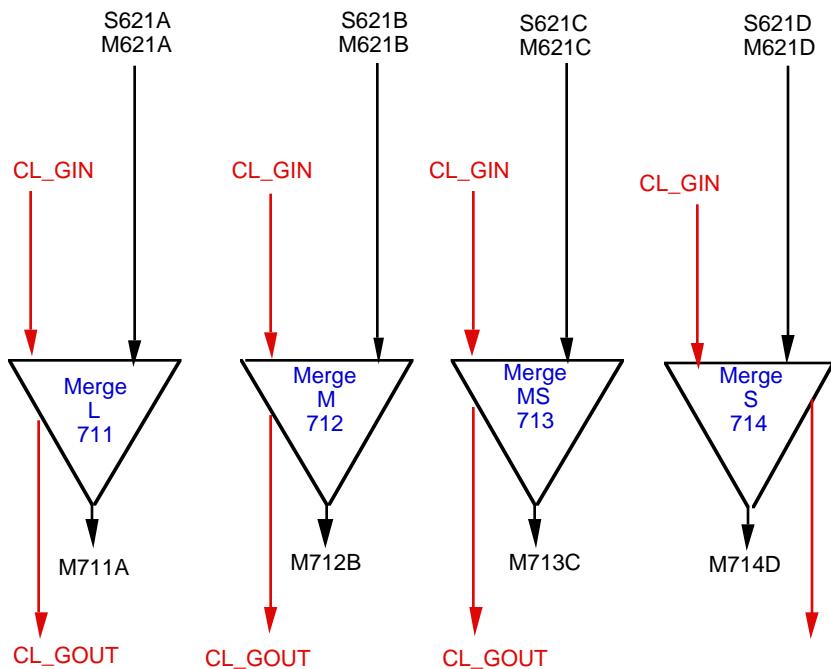


Figure B9. Plant Area 700 - Merge Recycle Particles.

Plant Area 800

In plant area 800 (Figure B10) recycled gas and oil streams are dealt with. In the process being simulated gases exiting the FBM and PYR are combined and then sent through a condensing system to drop out oil and water. Part of the oil is recycled to the PYR and most of the dry gas is reheated and used as fluidizing gas for the FBM and sweep gas for the PYR. In the simulation details of the condensation system are not dealt with, but the simulation of gas and oil recycle streams are accomplished. The first module in this area is two MERGE_STRMS modules used to combine all the gases exiting the FBM and PYR. Next, a PHASE_CHANGE module is used to drop out all of the three oil species used in the simulation. Liquid Oil-1 leaves the system while Oil-2 & 3 are sent on to a MERGE_STRMS and a SPLIT_STRMS

module where the desired flow rate of recycle oil is established. The temperature of the recycle stream is established by the previous PHASE_CHANGE module. The gas from the PHASE_CHANGE modules moves on to a SPLIT_STRMS module where the required flow of gas to feed the FBM is split off. The gas then passes to a MERGE_STRMS module where any nitrogen makeup gas is added. Finally, the gas passes through a PHASE_CHANGE modules which is used to heat the gas to the desired temperature to feed the FBM. The gas stream from the SPLIT_STRMS module goes to a second SPLIT_STRMS module where the required gas to feed the PYR is split off. The excess gas exits the system as the PYR_OUT stream. The PYR feed stream passes through a PHASE_CHANGE module which is used to heat the gas to the temperature required to feed the PYR.

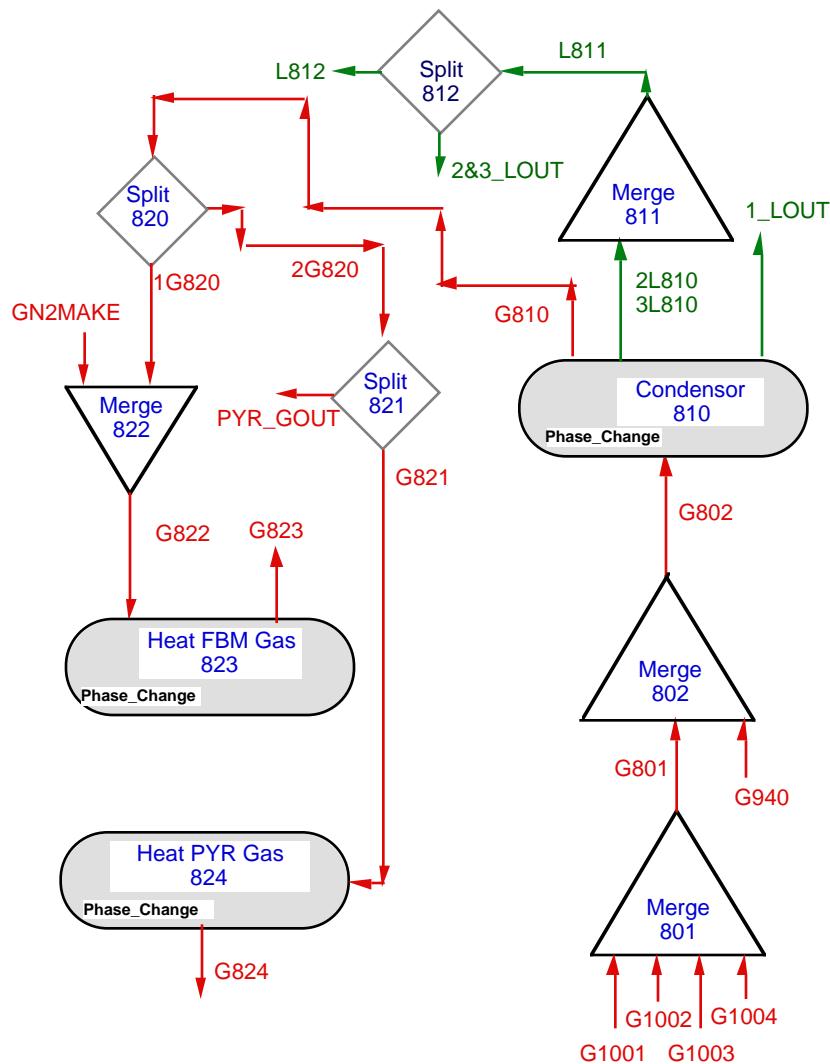


Figure B10. Plant Area 800 - Oil & Gas Recycle.

Plant Area 900

Modules in plant area 900 are used to simulate the operation of the FBM. The modules are shown schematically in Figure B11. The first module is a SPLIT_STRMS module which is used

to divide the flow in half to feed both sides of the FBM fluidized bed. The fluidized bed portion of the FBM is simulated using six FLUID_BED modules, three for each side of the bed. The fluidized beds are feed by recycled shale streams and by raw shale feed. Only the four non-fines streams enter the fluidized beds. The fines are assumed to pass immediately into and out of the head space of the unit.

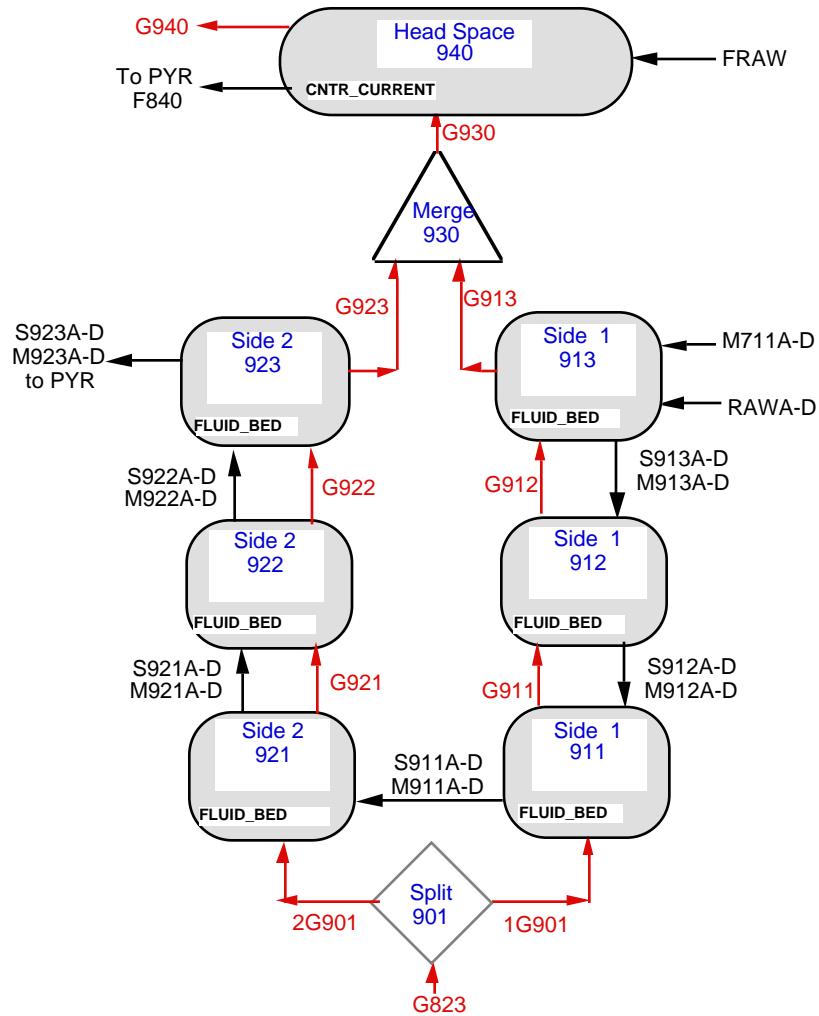


Figure B11. Plant Area 900 - FBM.

After the SPLIT_STRMS module the next module in the input file is the first FLUID_BED module on side one of the fluidized bed. Following this are the next five FLUID_BED modules following in order and proceeding in the direction of solid flow. Because the gas flow direction is counter current to the solids flow direction on side one, it is necessary to set the GASINIT parameter in the first two FLUID_BED modules so that they can be used to make an initial guess an injection gas flow to the module. In this simulation the gas stream at the bottom of the bed was used for this purpose since its flow rate is available at the time that the first computations of the FLUID_BED modules occur. On subsequent computational loops the GASINIT stream is not used since estimates of gas input streams are available from calculations done on earlier loops. As in the FBC modules particle size distributions in the

FLUID_BED modules are established as part of the input information. The same distribution is used for each of the FLUID_BED modules.

The FBM simulation is completed by using a MERGE_STRMS and CNTR_CURRENT module to simulate the FBM head space. The gas exiting the fluidized bed are merged by the MERGE_STRMS module and sent on to the CNTR_CURRENT module where they interact with the raw fines stream. In the CNTR_CURRENT module the particle velocity has been set, somewhat arbitrarily at 1 m/s. The CNTR_CURRENT module was chosen for the head space since it essentially simulates a dilute phase well mixed system.

Plant Area 1000

The final section of modules in the input file represent the PYR and are designated to be in plant area 1000 (Figure B12). The first three modules in this area are SPLIT_STRMS modules and are used to split up the gas flow to the modules used to simulated the moving packed bed pyrolyzer. Because the gas sweeps in a cross flow fashion through the bed, CSTR modules where chosen to simulated the bed. IBED and IDILUTE parameters are set to 2 so that correlations appropriate for dense phase systems are used in computing transport coefficients. After the SPLIT_STRMS modules the computations pass from one CSTR module to the next. Besides gas feed to the first CSTR, there is a flow of recycled liquid oil. To allow for a phase change in the unit, species and reaction flags have been added to the basic PYR set in this one module. These allow for the presence of the liquid oil and turn on the evaporation reactions for Oil-2 &3. The oil evaporation rate parameters have been set (in the \$PROPERTIES area) to insure that all the oil evaporates. Some care must be taken in setting these parameters. A rate high enough to insure essentially complete evaporation is desired, however, if the rates are set too high computational problems can arise. Some preliminary runs with a simple single module system were used to arrive at satisfactory values.

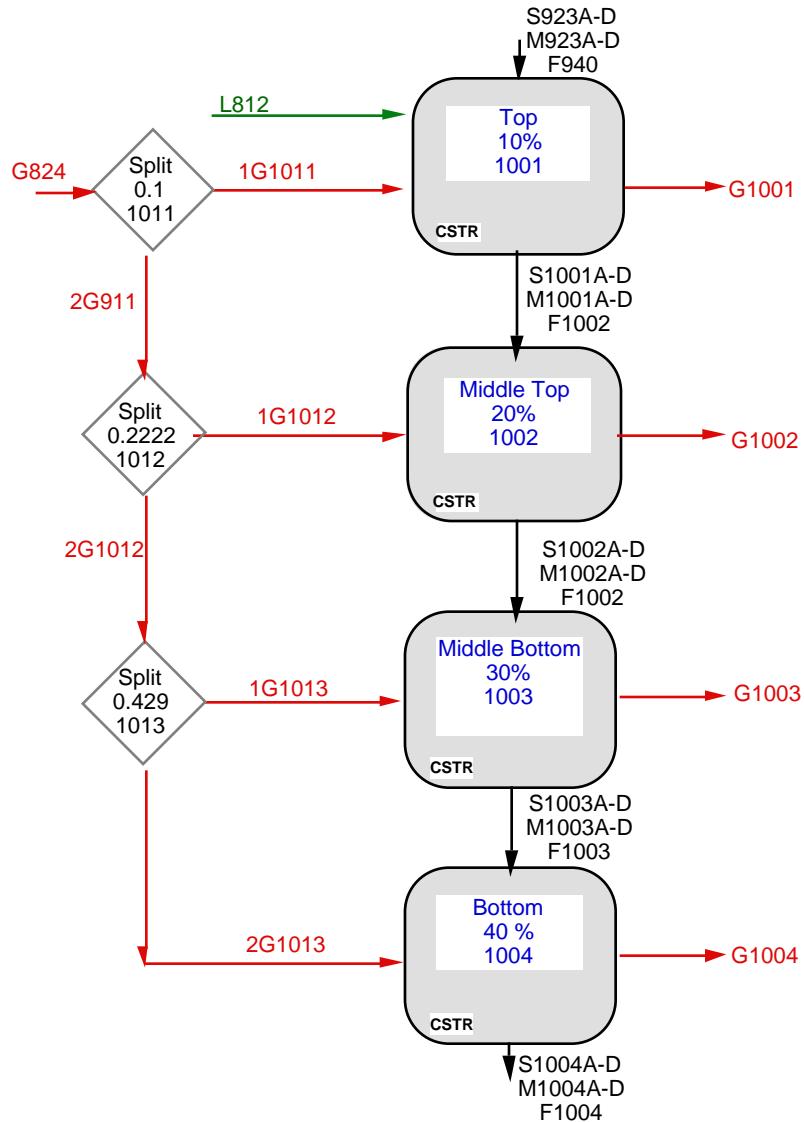


Figure B12. Plant Area 1000 - PYR.

This completes the module definition section of the input file. The final section deals with initialization of system stream variables. The number of initialized streams have been kept to a minimum to reduce the labor in changing to different operating conditions. Wide use of the systems ability to make initial guesses required to initiate solutions in reactor modules has been used.

Stream \$INIT's

The first three \$INITGAS entries initialize the gas input streams to the system. This is followed by definition of the artificial gas cooling stream used to set temperatures leaving the FBC. The final four \$INITGAS's set internal streams needed to allow the first computational loop to be completed. These are the streams which feed the gas and oil recycle modules into

area 800. Since modules in this plant area are executed before the FBM and PYR modules which generate them, it is necessary to make a reasonable guess for use in the first computation loop. In this case a guess is made which insures there will be enough gas and oil to feed the recycle streams.

Initialization of the solid streams make up the last entries in the input file. The first five \$INITSOLID entries define the rate and properties of the raw oil shale. The SAME_AS variable is used to avoid repeating information which applies to all raw solid streams. Only the flow and particle diameter are set in the last four entries. The location of the SAME_AS parameter relative to the FLOW and DIAM parameters is important because of the overwrite logic of the SAME_AS parameter. The final nine \$INITSOLID entries are an initial guess at the streams exiting the PYR. This is necessary since the computations start at the exit the PYR. Notice that all solid streams are set to the same values for PROP(1) & PROP(2). This was done since it is assumed all solids originated from a single grade of shale. The values of these properties were obtained from some preliminary simple OSP runs which accurately computed the needed densities of char and kerogen.

DESCRIPTION OF ASCII OUTPUT FILE

A listing of selected portions of the ASCII output file, the ".dat" file, are given in the last section in this Appendix. In this section a brief description of the file content is given.

After the title section the \$GLOBAL parameters in effect for the run are listed. The parameters are each listed beginning with the name used in the input file. This allows a more detailed explanation of their function to be found in the description of the input. Following the name some descriptive information set off in ":"'s may be present. After this the value of the parameter is listed. This general format is sometimes slightly modified to fit particular cases. An example is in the GROUP_LOOP(I) listing where the format after the name is specialized for this case.

After the \$GLOBAL parameters a longer section begins in which all \$PROPERTY parameters are listed. Again, these are the parameters in effect for the run. In this case this is identically the case. In general, however, it is possible that the stoichiometric coefficients listed here have been supplanted by results of a STOICH module calculation. In such a case the output from the STOICH modules should be consulted for any modification to values listed in this section. All parameters, reaction stoichiometry and species property parameters are listed in this section whether or not they are used in the simulation. Heat capacities and gas viscosities are functions of temperature and the coefficients used in computing their values are listed with column headings indicating the form of the term in which the coefficient is used.

Following the \$PROPERTIES section is a module by module list of parameters used for each invocation of a module in the input file. In the selected listing only a single module has been shown, a LIFT_PIPE module. For this module, as is the case for all modules, the connections are shown using the following abbreviations:

GI - for an input gas stream

GO - for an output gas stream
SI - for an input solid stream
SO - for an output gas stream
LI - for an input liquid stream (not present in this example)
LO - for an output liquid stream (not present in this example)
GB - for an internal gas bubble stream used by the FLUID_BED module

The pairing of solid input and output streams is determined by the order of their appearance in this list. For example in this case input stream S111A is paired with output stream S201A and input stream S112B is paired with output stream S201B, etc. The naming convention used causes some linkage in these names, through the ending letters, but it must be remembered that the module makes no use of this information.

Following the stream connections in the LIFT_PIPE module listing is a table which describes which species are active in the module. An active species has a number following it in the table. For solids there is a separate column for each active solid stream internal to the module, in this case there are nine such streams. The number following the active species is actually the ordering used by the module in the solution scheme and can be useful for debugging purposes.

Following the species table is a listing of the reactions which are active in the module. The numbers refer to their index number in the full list of reactions.

The final section of the LIFT_PIPE module input parameter listing gives other parameters used in the computations which can potentially be set by input values. In this case most of these values are default values.

The next area in the output file is a listing of all streams used in the simulation. The numbers associated with each name are the internal index used by the code to reference the particular stream. These references can be useful in certain debug operations. Following this section is a listing of internal stream numbers not used. This listing shows the number of streams available for future use.

Next a listing of potential connection problems determined by the code is shown. This listing includes all streams which have been used an odd number of times in module connection definitions. For overall input and output streams from the system an odd number is to be expected. Here the naming convention used, primarily non numeric names, allows the list to be scanned relatively easily for any real problems. In this case the list only includes actual overall system inlet and outlet streams.

The next section is a listing of convergence error values for each overall loop in the solution scheme. A loop is defined as one time through the computations of all modules present in the input file. The convergence errors are set by each individual module, but for the most part represent a scaled temperature. These are not errors made by the computations of the module but are the scaled difference between computed stream temperatures during the loop to those of the previous loop. For the case of the first loop the difference involves initial stream temperatures. The "Run times" shown are the total CPU time used by the simulation to that

point. The time associated with a loop is that at the end of the computations of that loop. The number printed before each module type are the tag numbers for the modules. The computations were judge by the code to converge after the 20th loop since all convergence errors were less than the convergence tolerance chosen for this problem of 0.0002.

The remainder of the output file consists of results listings generated by each module after overall convergence has been reached, in this case after the 21 loop. Only a few of the modules results are shown in the abbreviated listing. The first module shown is the LIFT_PIPE module which is simulating the 4TU-Pilot lift pipe. The first portion of the this module's output show the properties of all streams entering and leaving the module. Only those species which have been selected active for the module are shown. The values associated with the heading "Stream number" refer to the internal stream numbers used in the computations and the ASCII string "in" or "out" indicating whether the stream is entering or leaving a module. The three auxiliary properties, PROP(1), PROP(2) and PROP(3) are listed using the abbreviated labels, "O Chr kg/m**3" for PROP(1), "O Ker kg/m**3" for PROP(2), and "O FeS2 kg/m**3" for PROP(3). In the solid species area total weight fractions are listed for Kerogen's (although in this case only one kerogen has been used). The same summation is would also have been used for the individual Char species if they had been selected. However, in this simulation the overall composite Char species was used. Also note that the solid flow rates have been converted from input and internal units of kg/s units to kg/min units and the temperatures have been converted from degrees Kelvin to degrees Celsius. Small negative values of species compositions should be interpreted as zero. All modules use this same format to present information on streams associated with each particular module.

Following the stream information is a section describing overall elemental and energy balances for the module. This result is useful in insuring that the module computations have proceeded correctly and in determining overall processing in the module. Solid inorganic and organic weight fractions reported in this section are for the flow weighted average solid entering and leaving the module. For a satisfactory solution all fractional errors listed under the column headed by "(in-out)/average" should be small. How small can vary depending on the nature of the computations. For this LIFT_PIPE calculation these values are all quite small. However, in some cases they may be larger and still the computations can be considered satisfactory. The user needs to judge the basic nature of the changes occurring within the module and the magnitude of the flows of the atomic species. In some cases, when only trace amounts of a species is present, the fractional error can be relatively large, but depending on the circumstances, not reflect any serious problem with the results. In general, if the solution of a module fails there will be other indications. These balances serve only as a final double check. In certain cases the enthalpy balance can be used to gain additional information. For example in the PHASE_CHANGE module the enthalpy balance "in-out" is the heat effect associated with the phase and temperature changes occurring in the module.

For many modules the above information completes the output. However, for some modules there is additional information given. This is the case with the LIFT_PIPE module. The last section of the LIFT_PIPE output gives various computed parameters associated with the particle velocities in the lift. These velocities are reported for conditions at the inlet to the lift pipe and at the exit of the lift pipe. This is done since in the actual calculations the inlet

conditions are used to compute particle velocities. The difference in the two results give some indication of the error involved in this simplification. If difference are too large the module can be broken into a series of modules so that velocities in different sections of the lift pipe are more adequately represented. In this case the accuracy of the calculations is such that no subdivision of the physical lift pipe was used.

The next module output results shown are for the top 1/3 of the inlet side of the FBM. This is a FLUID_BED module. The stream data and overall balance results follow the format describe for the LIFT_PIPE module above. In addition to the inlet and outlet streams, the gas stream section includes a stream which has a "stream number" of "31 bub". This is an internal bubble stream and represents the properties of gas flowing in the bubble phase. In this case there is only one bubble called for in the input file. If more were called for, each bubble stream would appear with "bub" designation.

After the stream information output is present which gives additional information about the gas solid flow in the module. The effective particle size used in the fluidization calculations "dp*scale" is given. This is followed, in order, by the Archimedes' number, the minimum fluidization Reynolds number, the minimum fluidization velocity, the ratio of the overall gas superficial velocity to the minimum fluidization velocity, and the bubble velocity. The next portion of the output lists the parameters associated with the solid streams in the unit. The "Vol Frac" column is the fraction of the total volume occupied by solid in the unit which is associated with the listed stream. The mapping of the streams is on the basis of the order in which input solid streams are given in the output, which in turn is the same order they were listed in the input file. The last column "Res. Time" is the residence time of the particle in the unit. Note that particles of similar size have equal residence times. This is a result of the grouping of size classification which was specified in the input file.

The final section of this FLUID_BED module is the overall balance information described previously for the LIFT_PIPE module.

The last part of the output listing shown is that for output from the CSTR module which is used to simulate the top portion of the PYR bed. This output includes liquid streams which carry the recycled oil into the unit. Notice that essentially all the oil is evaporated. This was achieved by tuning on the evaporation parameters as mentioned previously. The CSTR output also includes information on the solid flows in the unit. In this case, since a moving packed bed is being simulated, the residence times for all solid streams are the same. This was achieved by omitting any particle size distribution information from the input for this module. In this case the module assumes uniform residence times for all streams based on the total solid throughput.

This completes the description of the example problem. The next two sections in this appendix give the listings of the input and output files. Although not discussed here, the user should remember to save the ".strm" file created during the run. This file is useful in restarting future similar simulations, obtaining summary information (see Appendix C), and obtaining detailed input for single unit simulations.

INPUT FILE

The following is a complete listing of the ASCII input file for this example problem.

```
$GLOBAL      loopmax=31    tol=2.0e-4   group_loop(1)=2
              title='Lab Retort H2O - 9P Sizes'

*****
*
* When performing a new run be sure to change/check following:
* (Note: All areas are flagged with 'DATA_n' so they can be
* readily located. The n is a key into comments below)
*
* 1. Set acitive coking area for rich or lean:
*     lean - 6e6,    rich - 2e6
*
* 2. Set the COMB-FBC $FLAG areas to reflect precence
*     or absence of oxygen in the FBC.
*
* 3. Set attrition (see results of at)
*     A. Raw fines after PYR
*     B. LFT fines after LFT
*     C. Breakage after DFC
*
* 4. Set particle size distributions in
*     A. FBC (2 units)
*     B. FBM (6 units)
*
* 5. Set solid recycle rates using recycle size distribution to
*     set individual rates
*
* 6. Set oil recyle temperature & rate
*
* 7. Set recycle gas flows & temperatures
*     A. FBM
*     B. PYR
*
* 8. Set injected gas flows, temperatures & compositions
*     A. LFT
*     B. FBC
*     C. N2 make to Pyrolysis side injection
*
* 9. Set cooling gas temperature
*
* 10. Review initial guess of gas out of FBM.
*
* 11. Set raw flow, temperature, composition & paricle sizes.
*
* 12. Review guess of single pass material out of PYR and
*     set flow compatable with raw rate.
*
* 13. Review guess of multiple pass material out of PYR and
*     set flow compatable with recycle rate.
*
* 14. Review requirement for oil evaporation in top PYR unit
*
*     *. Find all 'pres=' and set to average pressure
*
*-----
* Summary of where particle size information needed:
```

```

*
* Set to recycle size - Results of particle breakage, DATA_3C
* Multipass guess, DATA_13
*
* Set to fines free FBC size - FBC internal, DATA_4A
*
* Set to Raw size - Raw feed, DATA_11
* Single pass guess, DATA_12
*-----*
*****Available reactions, gases, liquids and solids.
*
* Reactions:
*   reaction='KER-1 + O2'      reaction='KER-2 + O2'
*   reaction='KER-3 + O2'      reaction='CHAR-C + O2'
*   reaction='CHAR-H + O2'      reaction='CHAR-O + O2'
*   reaction='CHAR-N + O2'      reaction='CHAR-S + O2'
*   reaction='MgCO3 DECOMP'    reaction='CaCO3 DECOMP'
*   reaction='KER-1 P L'        reaction='KER-1 P G'
*   reaction='OIL-1 ADS'       reaction='OIL-2 ADS'
*   reaction='OIL-3 ADS'       reaction='OIL-1 COK'
*   reaction='OIL-2 COK'       reaction='OIL-3 COK'
*   reaction='COKE + O2'       reaction='OIL-1 EVAP'
*   reaction='OIL-2 EVAP'      reaction='OIL-3 EVAP'
*   reaction='CHAR + O2'       reaction='FES2 COMB'
*   reaction='CaCO3 + SiO2'    reaction='EXTRA 1'
*   reaction='EXTRA 2'         reaction='EXTRA 3'
*   reaction='EXTRA 4'         '
*
* Gases:
*   gas='N2'                  gas='O2'          gas='H2'
*   gas='CO'                  gas='CO2'         gas='H2O'
*   gas='H2S'                 gas='SO2'         gas='NH3'
*   gas='NO2'                 gas='HCN'         gas='COS'
*   gas='CH4'                 gas='C2H4'        gas='C2H6'
*   gas='C3H6'                gas='C3H8'        gas='C5-pseudo'
*   gas='H12-pseudo'          gas='Oil-1'       gas='Oil-2'
*   gas='Oil-3'                gas='Oil-4'       gas='Oil-5'
*   gas='Gas-A'                gas='Gas-B'       gas='Gas-C'
*   gas='Gas-D'                '
*
* Liquids:
*   liq='Oil-1'                liq='Oil-2'       liq='Oil-3'
*   liq='Oil-4'                liq='Oil-5'       liq='Water'
*   liq='Liquid-A'             liq='Liquid-B'   '
*
* Solids:
*   sol(1)='Kerogen-1'         sol(1)='Kerogen-2'   sol(1)='Kerogen-3'
*   sol(1)='Char-C'            sol(1)='Char-H'     sol(1)='Char-O'
*   sol(1)='Char-N'            sol(1)='Char-S'     sol(1)='Inert'
*   sol(1)='Moisture'          sol(1)='Bound-water' sol(1)='CaCO3'
*   sol(1)='CaO'               sol(1)='CaSO4'      sol(1)='MgCO3'
*   sol(1)='MgO'               sol(1)='MgSO4'      sol(1)='CasIO3'
*   sol(1)='FeS2'              sol(1)='FeS'        sol(1)='Fe2O3'
*   sol(1)='SiO2'              sol(1)='N-inorganic' sol(1)='Oil-1'
*   sol(1)='Oil-2'              sol(1)='Oil-3'      sol(1)='Oil-4'
*   sol(1)='Oil-5'              sol(1)='Coke'       sol(1)='Char'
*   sol(1)='Solid-A'           sol(1)='Solid-B'    sol(1)='Solid-C'
*   sol(1)='Solid-D'           '
*
*****$PROPERTIES
```

```

sphericity=0.60

* Coking area (base 1.0e7)
solid_int = 1.0e7 m**2                                     DATA_1

* New coking kinetics (29-Jan-93)
a_coke(1)=1.7e7 a_coke(2)=1.7e7 a_coke(3)=1.7e7
t_coke(1)=16640 t_coke(2)=16640 t_coke(3)=16640
coke_rfac=0.3

* Use Sohn x about 3 oxidation rate. Use Sohn activation temperature
* Increase pre-exp by 3 to be consistant with Fujimoto data.
a_char_comb = 7 t_char_comb=11080
* Double coke rate by factor of 2 over char combustion rate.
a_coke_comb =14 t_coke_comb=11080

* Set oil evaporation constant to make solution easier
a_evap(2)=1.0e-4 a_evap(3)=1.0e-4

*****
* Set global flags for use by modules.
*****


$FLAGREAC = COMB
reaction='KER-1 + O2'           reaction='COKE + O2'
reaction='CHAR + O2'
reaction='CACO3 DECOMP'         reaction='MGC03 DECOMP'
reaction='CACO3 + SIO2'
reaction='OIL-1 COK'            reaction='OIL-2 COK'
reaction='OIL-3 COK'

$FLAGGAS = COMB
gas='N2'                      gas='O2'                  gas='H2'
gas='CO2'                     gas='H2O'                 gas='H2S'
gas='SO2'                     gas='NH3'                 gas='NO2'
gas='CH4'                     gas='C2H4'                gas='C3H6'
gas='Oil-1'                   gas='Oil-2'               gas='Oil-3'

$FLAGSOLID = COMB
sol(1)='Kerogen-1'             sol(1)='Char'              sol(1)='Coke'
sol(1)='Inert'                 sol(1)='SiO2'               sol(1)='CaSiO3'
sol(1)='CaCO3'                 sol(1)='CaO'                 sol(1)='MgO'
sol(1)='MgCO3'                 sol(1)='Oil-2'               sol(1)='Oil-3'

*****
$FLAGREAC = COMB-FBC          DATA_2
reaction='COKE + O2'           reaction='CHAR + O2'
reaction='CACO3 DECOMP'         reaction='MGC03 DECOMP'
reaction='CACO3 + SIO2'

$FLAGGAS   = COMB-FBC          DATA_2
gas='N2'                      gas='O2'
gas='CO2'                     gas='H2O'
gas='SO2'                     gas='NO2'

$FLAGSOLID = COMB-FBC
sol(1)='Inert'                 sol(1)='Char'              sol(1)='Coke'
sol(1)='CaCO3'                 sol(1)='SiO2'               sol(1)='CaSiO3'

```

```

sol(1)='MgCO3'           sol(1)='MgO'

*****
$FLAGREAC = PYR
reaction='KER-1 P G'
reaction='CACO3 DECOMP'   reaction='MGC03 DECOMP'
reaction='CACO3 + SIO2'
reaction='OIL-1 ADS'      reaction='OIL-2 ADS'
reaction='OIL-3 ADS'
reaction='OIL-1 COK'      reaction='OIL-2 COK'
reaction='OIL-3 COK'

$FLAGGAS = PYR
gas='N2'                  gas='H2'                  gas='CO2'
gas='H2O'                 gas='H2S'                 gas='NH3'
gas='CH4'                 gas='C2H4'                gas='C3H6'
gas='Oil-1'                gas='Oil-2'                gas='Oil-3'

$FLAGSOLID = PYR
sol(1)='Kerogen-1'        sol(1)='Char'               sol(1)='Coke'
sol(1)='Inert'             sol(1)='SiO2'               sol(1)='Casio3'
sol(1)='CaCO3'             sol(1)='CaO'                 sol(1)='Oil-3'
sol(1)='MgCO3'             sol(1)='MgO'                 sol(1)='Oil-2'
sol(1)='Oil-1'              sol(1)='Oil-1'               sol(1)='Oil-3'

*****
* Module definition section. Keywords required (no spaces in keywords).
*****



*##### Pass Thru (for Loop Isolation) #####
$MODULE = PASS_THRU desc='Isolate Loop'
tag='101'
print=0
si=S1004A  so=S101A
si=S1004B  so=S101B
si=S1004C  so=S101C
si=S1004D  so=S101D
si=M1004A  so=M101A
si=M1004B  so=M101B
si=M1004C  so=M101C
si=M1004D  so=M101D
si=F1004   so=F101

*##### End Pass Thru #####

```

```

*##### Pyrolyzer Attrition Train #####
*****  

$MODULE = RELAX      desc= 'Relax out of Main Pyrolyzer'  

                     tag='102'  

                     relax=1.00  

                     solidin=S101A  solidout=S102A  

                     solidin=S101B  solidout=S102B  

                     solidin=S101C  solidout=S102C  

                     solidin=S101D  solidout=S102D  

                     solidin=F101   solidout=F102  

*****  

$MODULE = ATTRITION    desc= 'After Pyrolyzer S-L to fines'  

                     tag='111'  

                     si=S102A  type=4  

                     so(1)=S111A  

                     so(2)=F111   split=0.08  newdiam=0.00005           DATA_3A  

*****  

$MODULE = ATTRITION    desc= 'After Pyrolyzer S-M to fines'  

                     tag='112'  

                     si=S102B  type=4  

                     so(1)=S112B  

                     so(2)=F112   split=0.08  newdiam=0.00005           DATA_3A  

*****  

$MODULE = ATTRITION    desc= 'After Pyrolyzer S-MS to fines'  

                     tag='113'  

                     si=S102C  type=4  

                     so(1)=S113C  

                     so(2)=F113   split=0.08  newdiam=0.00005           DATA_3A  

*****  

$MODULE = ATTRITION    desc= 'After Pyrolyzer S-S to fines'  

                     tag='114'  

                     si=S102D  type=4  

                     so(1)=S114D  

                     so(2)=F114   split=0.08  newdiam=0.00005           DATA_3A  

*****  

$MODULE = MERGE_STRMS  desc= 'From Pyrolyzer Attrition (F)'  

                     tag='120'  

                     so(1)=F120  

                     si(1)=F111  si(1)=F112  si(1)=F113  si(1)=F114  si(1)=F102  

*****  

*##### End Pyrolyzer Attrition Train #####
*****  

*##### Lift Pipe Train #####
*****  

$MODULE = LIFT_PIPE    desc= 'Lift Pipe'  

                     tag='201'  

                     gasin=LFT_GIN  gasout=G201  

                     solidin=S111A  solidin=S112B  solidin=S113C  solidin=S114D  

                     solidin=M101A  solidin=M101B  solidin=M101C  solidin=M101D  

                     solidin=F120  

                     solidout=S201A solidout=S201B solidout=S201C solidout=S201D  

                     solidout=M201A solidout=M201B solidout=M201C solidout=M201D  

                     solidout=F201  

                     diameter=0.057 m height = 9.2 m  

                     del_coke_comb=0.02

```

```

gas_flags=COMB    sol_flags(1)=COMB    reac_flags=COMB
solsame=1

*#####
*##### End Lift Pipe Train #####
*#####

*#####
*##### Lift Pipe Attrition Train #####
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (S-L)'
tag='301'
si=S201A type=6
so(1)=S301A
so(2)=F301 ashdiam=0.00005   split=0.16          DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (S-M)'
tag='302'
si=S201B type=6
so(1)=S302B
so(2)=F302 ashdiam=0.00005   split=0.14          DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (S-MS)'
tag='303'
si=S201C type=6
so(1)=S303C
so(2)=F303 ashdiam=0.00005   split=0.02          DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (S-S)'
tag='304'
si=S201D type=6
so(1)=S304D
so(2)=F304 ashdiam=0.00005   split=0.0          DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (M-L)'
tag='321'
si=M201A type=6
so(1)=M321A
so(2)=F321 ashdiam=0.00005   split=0.020         DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (M-M)'
tag='322'
si=M201B type=6
so(1)=M322B
so(2)=F322 ashdiam=0.00005   split=0.020         DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (M-MS)'
tag='323'
si=M201C type=6
so(1)=M323C
so(2)=F323 ashdiam=0.00005   split=0.005         DATA_3B
*****$MODULE = ATTRITION      desc= 'After Lift Pipe (M-S)'
tag='324'
si=M201D type=6
so(1)=M324D
so(2)=F324 ashdiam=0.00005   split=0.0          DATA_3B

```

```

*****
$MODULE = MERGE_STRMS desc ='Merge all Multipass Lift Pipe fines'
tag='330'
so(1)=F330
si(1)=F321 si(1)=F322 si(1)=F323 si(1)=F324

*****
$MODULE = MERGE_STRMS desc ='Merge all Lift Pipe fines'
tag='310'
so(1)=F310
si(1)=F301 si(1)=F302 si(1)=F303 si(1)=F304
si(1)=F201 si(1)=F330

*##### End Lift Pipe Train #####
*##### Delayed Fall Combustor Train #####
*****  

$MODULE = CO_CURRENT desc= 'Delayed Fall Combustor'
tag='401'
gasin=G201 gasout=G401
solidin=S301A solidin=S302B solidin=S303C solidin=S304D
solidin=M321A solidin=M322B solidin=M323C solidin=M324D
solidin=F310
solidout=S401A solidout=S401B solidout=S401C solidout=S401D
solidout=M401A solidout=M401B solidout=M401C solidout=M401D
solidout=F401
diameter = 0.133 m height = 3.0 m
idilute=1 ibed=1

velp(1)=0.5 velp(2)=0.5 velp(3)=0.5 velp(4)=0.5
velp(5)=0.5 velp(6)=0.5 velp(7)=0.5 velp(8)=0.5
velp(9)=2.0

gas_flags=COMB sol_flags(1)=COMB reac_flags=COMB
solsame=1

*****  

$MODULE = LIFT_PIPE desc= 'DFC Annulus'
tag='402'
gasin=G401 gasout=DFC_GOUT
solidin=F401
solidout=DFC_FOUT
diameter = 0.16 m height = 3 m
vslipcalc = 0

vslip(1) = 0.08 (fines)

gas_flags=COMB sol_flags(1)=COMB reac_flags=COMB
solsame=1

*****  

*##### End Delayed Fall Lift Combustor Train #####
*##### Start Particle Breakup Train #####
*****  

$MODULE = ATTRITION desc= 'Break S-L Particles'
tag='501'

```

```

        si=S401A type=1
        so(1)=S501A split(1)=0.668   newdiam(1)=-1.0          DATA_3C
        so(2)=S501B split(2)=0.157   newdiam(2)=0.0035  Medium
        so(3)=S501C split(3)=0.175   newdiam(3)=0.0017  Medium-small

*****
$MODULE = ATTRITION    desc= 'Break S-M Particles'
                    tag='502'
        si=S401B type=1
        so(1)=S502B split(1)=0.692   newdiam(1)=-1.0          DATA_3C
        so(2)=S502C split(2)=0.256   newdiam(2)=0.0017  Medium-small
        so(3)=S502D split(3)=0.052   newdiam(3)=0.0004  Small

*****
$MODULE = ATTRITION    desc= 'Break S-MS Particles'
                    tag='503'
        si=S401C type=1
        so(1)=S503C split(1)=0.732   newdiam(1)=-1.0          DATA_3C
        so(2)=S503D split(2)=0.268   newdiam(2)=0.0004  Small

*****
$MODULE = MERGE_STRMS  desc = 'Merge S-M After Breakage'
                    tag='512'
        so(1)=S512B
        si(1)=S501B  si(1)=S502B

*****
$MODULE = MERGE_STRMS  desc = 'Merge S-MS After Breakage'
                    tag='513'
        so(1)=S513C
        si(1)=S501C  si(1)=S502C  si(1)=S503C

*****
$MODULE = MERGE_STRMS  desc = 'Merge S-S After Breakage'
                    tag='514'
        so(1)=S514D
        si(1)=S502D  si(1)=S503D  si(1)=S401D

*****
$MODULE = ATTRITION    desc= 'Break M-L Particles'
                    tag='521'
        si=M401A type=1
        so(1)=M521A split(1)=0.960   newdiam(1)=-1.0          DATA_3C
        so(2)=M521B split(2)=0.019   newdiam(2)=0.0035
        so(3)=M521C split(3)=0.021   newdiam(3)=0.0017

*****
$MODULE = ATTRITION    desc= 'Break M-M Particles'
                    tag='522'
        si=M401B type=1
        so(1)=M522B split(1)=0.956   newdiam(1)=-1.0          DATA_3C
        so(2)=M522C split(2)=0.037   newdiam(2)=0.0017
        so(3)=M522D split(3)=0.007   newdiam(3)=0.0004

*****
$MODULE = ATTRITION    desc= 'Break M-MS Particles'
                    tag='523'
        si=M401C type=1
        so(1)=M523C split(1)=0.920   newdiam(1)=-1.0          DATA_3C
        so(2)=M523D split(2)=0.080   newdiam(2)=0.0004

*****
$MODULE = MERGE_STRMS  desc = 'Merge M-M After Breakage'

```

```

tag='532'
so(1)=M532B
si(1)=M521B si(1)=M522B

*****$MODULE = MERGE_STRMS desc = 'Merge M-MS After Breakage'
tag='533'
so(1)=M533C
si(1)=M521C si(1)=M522C si(1)=M523C

*****$MODULE = MERGE_STRMS desc = 'Merge M-S After Breakage'
tag='534'
so(1)=M534D
si(1)=M522D si(1)=M523D si(1)=M401D

*##### End Particle Breakup Train #####
*##### Fluid Bed Combustor Train #####
*****$MODULE = CSTR      desc= 'Fluidized Bed Combustor 1'
tag='601'
group=1
gasin=G630   gasout=FBC_GOUT   gasinit=FBC_GIN
solidin=S501A solidin=S512B solidin=S513C solidin=S514D
solidin=M521A solidin=M532B solidin=M533C solidin=M534D
solidout=S601A solidout=S601B solidout=S601C solidout=S601D
solidout=M601A solidout=M601B solidout=M601C solidout=M601D
diameter = 0.15 m height = 0.18 m
bedporosity = 0.61
DATA_4A
pdist_vf(1)=0.36 pdist_strm(1)=S501A pdist_strm(1)=M521A
pdist_vf(2)=0.44 pdist_strm(2)=S512B pdist_strm(2)=M532B
pdist_vf(3)=0.18 pdist_strm(3)=S513C pdist_strm(3)=M533C
pdist_vf(4)=0.02 pdist_strm(4)=S514D pdist_strm(4)=M534D
rtol=1.0e-4

gas_flags=COMB-FBC sol_flags(1)=COMB-FBC reac_flags=COMB-FBC
solsame=1

*** Recycle rate 5.8 kg/min = 0.097 kg/s
*****$MODULE = SPLIT_STRMS desc= 'Control Solid Recycle - L'
tag='611'
group=1
ssplit=0.0349 kg/s 36% DATA_5
si=S601A so(1)=S611A so(2)=SA_SOUT
si=M601A so(1)=M611A so(2)=MA_SOUT

*****$MODULE = SPLIT_STRMS desc= 'Control Solid Recycle - M'
tag='612'
group=1
ssplit=0.0427 kg/s 44% DATA_5
si=S601B so(1)=S612B so(2)=SB_SOUT
si=M601B so(1)=M612B so(2)=MB_SOUT

*****$MODULE = SPLIT_STRMS desc= 'Control Solid Recycle - MS'
tag='613'
group=1

```

```

ssplit=0.0175 kg/s    18%          DATA_5
si=S601C so(1)=S613C so(2)=SC_SOUT
si=M601C so(1)=M613C so(2)=MC_SOUT

*****$MODULE = SPLIT_STRMS desc= 'Control Solid Recycle - S'
tag='614'
group=1
ssplit=0.0019 kg/s    2%          DATA_5
si=S601D so(1)=S614D so(2)=SD_SOUT
si=M601D so(1)=M614D so(2)=MD_SOUT

*****$MODULE = CSTR      desc= 'Fluidized Bed Combustor 2'
tag='621'
group=1
gasin=FBC_GIN  gasout=G621
solidin=S611A  solidin=S612B  solidin=S613C  solidin=S614D
solidin=M611A  solidin=M612B  solidin=M613C  solidin=M614D
solidout=S621A solidout=S621B solidout=S621C solidout=S621D
solidout=M621A solidout=M621B solidout=M621C solidout=M621D
diameter = 0.15 m height = 0.37 m
bedporosity = 0.60          DATA_4A
pdist_vf(1)=0.36 pdist_strm(1)=S611A pdist_strm(1)=M611A
pdist_vf(2)=0.44 pdist_strm(2)=S612B pdist_strm(2)=M612B
pdist_vf(3)=0.18 pdist_strm(3)=S613C pdist_strm(3)=M613C
pdist_vf(4)=0.02 pdist_strm(4)=S614D pdist_strm(4)=M614D
rtol=1.0e-4

gas_flags=COMB-FBC  sol_flags(1)=COMB-FBC  reac_flags=COMB-FBC
solsame=1

*****$MODULE = MERGE_STRMS desc= 'Error check for FBC gas'
tag='630'
gi=G621      go=G630

*##### End Fluid Bed Combustor Train #####
*##### FBC Particle Merge & Cooling #####
*****$MODULE = MERGE_STRMS desc= 'Merge Recycled Particles & Cool - L'
tag='711'
so(1)=M711A  si(1)=S621A  si(1)=M621A
gi=CL_GIN   go=CL_GOUT

*****$MODULE = MERGE_STRMS desc= 'Merge Recycled Particles & Cool - M'
tag='712'
so(1)=M712B  si(1)=S621B  si(1)=M621B
gi=CL_GIN   go=CL_GOUT

*****$MODULE = MERGE_STRMS desc= 'Merge Recycled Particles & Cool - MS'
tag='713'
so(1)=M713C  si(1)=S621C  si(1)=M621C
gi=CL_GIN   go=CL_GOUT

```

```

*****
$MODULE = MERGE_STRMS desc= 'Merge Recyled Particles & Cool - S'
      tag='714'
      so(1)=M714D si(1)=S621D si(1)=M621D
      gi=CL_GIN go=CL_GOUT

***** End FBC Particle Merge & Cooling #####
***** Oil & Gas Recycle Train #####
*****



***** $MODULE = MERGE_STRMS desc= 'Merge Gas from PYR'
      tag='801'
      go=G801    gi=G1001   gi=G1002   gi=G1003   gi=G1004

***** $MODULE = MERGE_STRMS desc= 'Merge Gas from FBM & PYR'
      tag='802'
      go=G802    gi=G801   gi=G940

***** $MODULE = PHASE_CHANGE desc= 'Condense All Oils'
      tag='810'
      type=C temp=415 (This serves as oil reinjection temp.) DATA_6
      gi=G802 go=G810 lo=1_LOUT lo=2L810 lo=3L810
      gas=oil-1 gas=oil-2 gas=oil-3

***** $MODULE = MERGE_STRMS desc= 'Merge Condensed Oils 2&3'
      tag='811'
      lo=L811 li=2L810 li=3L810

***** $MODULE = SPLIT_STRMS desc= 'Control OIL Recycle'
      tag='812'
      lsplit=0.0025 kg/s (150 g/min)           DATA_6
      li=L811 lo=L812 lo=2&3_LOUT

***** $MODULE = SPLIT_STRMS desc= 'Get FBM Recycle Gas'
      tag='820'
      gsplit=0.76 mol/s                         DATA_7A
      gi=G810 go=1G820 go=2G820

***** $MODULE = MERGE_STRMS desc= 'Add N2 from L-valves & Bleed To FBM'
      tag='822'
      go=G822 gi=1G820 gi=GN2MAKE

*****


$MODULE = PHASE_CHANGE desc= 'Heat FBM Injected Gas'
      tag='823'
      type=C temp=772                           DATA_7A
      gi=G822 go=G823

***** $MODULE = SPLIT_STRMS desc= 'Get PYR Recycle Gas'
      tag='821'
      gsplit=0.064 mol/s                      DATA_7B
      gi=2G820 go=G821 go=PYR_GOUT

***** $MODULE = PHASE_CHANGE desc= 'Heat PYR Injected Gas'

```

```

tag='824'
type=C temp=772                               DATA_7B
gi=G821 go=G824

*#####End Oil & Gas Recycle Train #####
*##### Mixer Train #####
*****$MODULE = SPLIT_STRMS desc= 'Mixer Gas Feed'
tag='901'
gsplit=-0.5
gi=G823 go=1G901 go=2G901
*****
$MODULE = FLUID_BED desc= 'Mixer Side 1 Top'
tag='913'
gasin=G912 gasout=G913 gasinit=1G901
solidin=RAWA solidin=RAWB solidin=RAWC solidin=RAWD
solidin=M711A solidin=M712B solidin=M713C solidin=M714D
solidout=S913A solidout=S913B solidout=S913C solidout=S913D
solidout=M913A solidout=M913B solidout=M913C solidout=M913D
diameter = 0.105 m height = 0.137 m
                                                DATA_4A
pdist_vf(1)=0.49 pdist_strm(1)=RAWA pdist_strm(1)=M711A
pdist_vf(2)=0.35 pdist_strm(2)=RAWB pdist_strm(2)=M712B
pdist_vf(3)=0.13 pdist_strm(3)=RAWC pdist_strm(3)=M713C
pdist_vf(4)=0.03 pdist_strm(4)=RAWD pdist_strm(4)=M714D
rtol=1.0e-4
nbub = 1

gas_flags=PYR sol_flags(1)=PYR reac_flags=PYR
solsame=1
*****
$MODULE = FLUID_BED desc= 'Mixer Side 1 Middle'
tag='912'
gasin=G911 gasout=G912 gasinit=1G901
solidin=S913A solidin=S913B solidin=S913C solidin=S913D
solidin=M913A solidin=M913B solidin=M913C solidin=M913D
solidout=S912A solidout=S912B solidout=S912C solidout=S912D
solidout=M912A solidout=M912B solidout=M912C solidout=M912D
diameter = 0.105 m height = 0.137 m
                                                DATA_4A
pdist_vf(1)=0.49 pdist_strm(1)=S913A pdist_strm(1)=M913A
pdist_vf(2)=0.35 pdist_strm(2)=S913B pdist_strm(2)=M913B
pdist_vf(3)=0.13 pdist_strm(3)=S913C pdist_strm(3)=M913C
pdist_vf(4)=0.03 pdist_strm(4)=S913D pdist_strm(4)=M913D
rtol=1.0e-4
nbub = 1

gas_flags=PYR sol_flags(1)=PYR reac_flags=PYR
solsame=1
*****
$MODULE = FLUID_BED desc= 'Mixer Side 1 Bottom'
tag='911'
gasin=1G901 gasout=G911
solidin=S912A solidin=S912B solidin=S912C solidin=S912D
solidin=M912A solidin=M912B solidin=M912C solidin=M912D
solidout=S911A solidout=S911B solidout=S911C solidout=S911D
solidout=M911A solidout=M911B solidout=M911C solidout=M911D
diameter = 0.105 m height = 0.137 m

```

```

                                DATA_4A
pdist_vf(1)=0.49  pdist_strm(1)=S912A  pdist_strm(1)=M912A
pdist_vf(2)=0.35  pdist_strm(2)=S912B  pdist_strm(2)=M912B
pdist_vf(3)=0.13  pdist_strm(3)=S912C  pdist_strm(3)=M912C
pdist_vf(4)=0.03  pdist_strm(4)=S912D  pdist_strm(4)=M912D
rtol=1.0e-4
nbub = 1

gas_flags=PYR  sol_flags(1)=PYR  reac_flags=PYR
solsame=1

*****
$MODULE = FLUID_BED    desc= 'Mixer Side 2 Bottom'
tag='921'
gasin=2G901      gasout=G921
solidin=S911A    solidin=S911B    solidin=S911C    solidin=S911D
solidin=M911A    solidin=M911B    solidin=M911C    solidin=M911D
solidout=S921A   solidout=S921B   solidout=S921C   solidout=S921D
solidout=M921A   solidout=M921B   solidout=M921C   solidout=M921D
diameter = 0.105 m height = 0.137 m
                                DATA_4A
pdist_vf(1)=0.49  pdist_strm(1)=S911A  pdist_strm(1)=M911A
pdist_vf(2)=0.35  pdist_strm(2)=S911B  pdist_strm(2)=M911B
pdist_vf(3)=0.13  pdist_strm(3)=S911C  pdist_strm(3)=M911C
pdist_vf(4)=0.03  pdist_strm(4)=S911D  pdist_strm(4)=M911D
rtol=1.0e-4
nbub = 1

gas_flags=PYR  sol_flags(1)=PYR  reac_flags=PYR
solsame=1

*****
$MODULE = FLUID_BED    desc= 'Mixer Side 2 Middle'
tag='922'
gasin=G921      gasout=G922
solidin=S921A    solidin=S921B    solidin=S921C    solidin=S921D
solidin=M921A    solidin=M921B    solidin=M921C    solidin=M921D
solidout=S922A   solidout=S922B   solidout=S922C   solidout=S922D
solidout=M922A   solidout=M922B   solidout=M922C   solidout=M922D
diameter = 0.105 m height = 0.137 m
                                DATA_4A
pdist_vf(1)=0.49  pdist_strm(1)=S921A  pdist_strm(1)=M921A
pdist_vf(2)=0.35  pdist_strm(2)=S921B  pdist_strm(2)=M921B
pdist_vf(3)=0.13  pdist_strm(3)=S921C  pdist_strm(3)=M921C
pdist_vf(4)=0.03  pdist_strm(4)=S921D  pdist_strm(4)=M921D
rtol=1.0e-4
nbub = 1

gas_flags=PYR  sol_flags(1)=PYR  reac_flags=PYR
solsame=1

*****
$MODULE = FLUID_BED    desc= 'Mixer Side 2 Top'
tag='923'
gasin=G922      gasout=G923
solidin=S922A    solidin=S922B    solidin=S922C    solidin=S922D
solidin=M922A    solidin=M922B    solidin=M922C    solidin=M922D
solidout=S923A   solidout=S923B   solidout=S923C   solidout=S923D
solidout=M923A   solidout=M923B   solidout=M923C   solidout=M923D
diameter = 0.105 m height = 0.137 m
                                DATA_4A

```

```

pdist_vf(1)=0.49  pdist_strm(1)=S922A  pdist_strm(1)=M922A
pdist_vf(2)=0.35  pdist_strm(2)=S922B  pdist_strm(2)=M922B
pdist_vf(3)=0.13  pdist_strm(3)=S922C  pdist_strm(3)=M922C
pdist_vf(4)=0.03  pdist_strm(4)=S922D  pdist_strm(4)=M922D
rtol=1.0e-4
nbub = 1

gas_flags=PYR  sol_flags(1)=PYR  reac_flags=PYR
solsame=1

*****
$MODULE = MERGE_STRMS desc= 'Merge Mixer Gases'
tag='930'
go(1)=G930 gi(1)=G913  gi(1)=G923

*****
$MODULE = CNTR_CURRENT desc= 'Mixer Head Space'
tag='940'
gasin=G930 gasout=G940
solidin=FRAW
solidout=F940
diameter = 0.2 m height = 0.91 m
ibed=1 idilute=1
rtol=1.0e-4

velp(1)=1.0 m/s

gas_flags=PYR  sol_flags(1)=PYR  reac_flags=PYR
solsame=1

***** End Mixer Train *****

***** Pyrolyzer Train *****

*****
$MODULE = SPLIT_STRMS desc= 'Pyrolyzer Gas Feed'          print=0
tag='1011'
gsplit=-0.1
gi=G824  go=1G1011  go=2G1011

*****
$MODULE = SPLIT_STRMS desc= 'Pyrolyzer Gas Feed'          print=0
tag='1012'
gsplit=-0.2222
gi=2G1011  go=1G1012  go=2G1012

*****
$MODULE = SPLIT_STRMS desc= 'Pyrolyzer Gas Feed'          print=0
tag='1013'
gsplit=-0.429
gi=2G1012  go=1G1013  go=2G1013

*****
$MODULE = CSTR      desc= 'Pyrolyzer Top'
tag='1001'
gasin=1G1011      gasout=G1001
liqin=L812        liqout=LDUM
solidin=S923A     solidin=S923B  solidin=S923C  solidin=S923D
solidin=M923A     solidin=M923B  solidin=M923C  solidin=M923D
solidin=F940
solidout=S1001A    solidout=S1001B  solidout=S1001C  solidout=S1001D
solidout=M1001A    solidout=M1001B  solidout=M1001C  solidout=M1001D

```

```

solidout=F1001
diameter = 0.2 m height = 0.085 m
rtol=1.0e-5
ibed=2 idilute=2
bedporosity = 0.45

gas_flags=PYR sol_flags(1)=PYR reac_flags=PYR
liq='OIL-2' liq='OIL-3' DATA_14
reaction='OIL-2 EVAP' reaction='OIL-3 EVAP'
solsame=1

*****
$MODULE = CSTR desc= 'Pyrolyzer Middle Top'
tag='1002'
gasin=1G1012 gasout=G1002
solidin=S1001A solidin=S1001B solidin=S1001C solidin=S1001D
solidin=M1001A solidin=M1001B solidin=M1001C solidin=M1001D
solidin=F1001
solidout=S1002A solidout=S1002B solidout=S1002C solidout=S1002D
solidout=M1002A solidout=M1002B solidout=M1002C solidout=M1002D
solidout=F1002
diameter = 0.2 m height = 0.17 m
ibed=2 idilute=2
rtol=1.0e-4
bedporosity = 0.45

gas_flags=PYR sol_flags(1)=PYR reac_flags=PYR
solsame=1

*****
$MODULE = CSTR desc= 'Pyrolyzer Middle Bottom'
tag='1003'
gasin=1G1013 gasout=G1003
solidin=S1002A solidin=S1002B solidin=S1002C solidin=S1002D
solidin=M1002A solidin=M1002B solidin=M1002C solidin=M1002D
solidin=F1002
solidout=S1003A solidout=S1003B solidout=S1003C solidout=S1003D
solidout=M1003A solidout=M1003B solidout=M1003C solidout=M1003D
solidout=F1003
diameter = 0.2 m height = 0.255 m
rtol=1.0e-4
ibed=2 idilute=2
bedporosity = 0.45

gas_flags=PYR sol_flags(1)=PYR reac_flags=PYR
solsame=1

*****
$MODULE = CSTR desc= 'Pyrolyzer Bottom'
tag='1004'
gasin=2G1013 gasout=G1004
solidin=S1003A solidin=S1003B solidin=S1003C solidin=S1003D
solidin=M1003A solidin=M1003B solidin=M1003C solidin=M1003D
solidin=F1003
solidout=S1004A solidout=S1004B solidout=S1004C solidout=S1004D
solidout=M1004A solidout=M1004B solidout=M1004C solidout=M1004D
solidout=F1004
diameter = 0.2 m height = 0.34 m
rtol=1.0e-4
ibed=2 idilute=2
bedporosity = 0.45

```

```

gas_flags=PYR    sol_flags(1)=PYR    reac_flags=PYR
solsame=1

*#####
* Pyrolyzer End #####
***** Stream initialization section. Keywords required. *****
(For ease of editing do not use blanks in value definitions.)

*#####
* Gases #####
*#####
* Injected #####
***** Into Lift Pipes DATA_8A
$INITGAS=LFT_GIN flow=0.603 mol/s temp=773 K pres=157.0e3 Pa
o2=0.21 n2=0.79

***** Into Fluid Bed Combustor DATA_8B
$INITGAS=FBC_GIN flow=0.441 mol/s temp=873 K pres=157.0e3 Pa
o2=0.073 n2=0.927

***** N2 Make Into Fluid Bed Mixer (RPH flow + LVC flow + 1/2 Bleed) DATA_8C
(Temp is average of inflows)
$INITGAS=GN2MAKE flow=0.166 mol/s temp=584 K pres=157.0e3 Pa
n2=1.0

*#####
* Injected (but not into units) #####
***** Cooling Gas DATA_9
$INITGAS=CL_GIN flow=1000 mol/s temp=970 K pres=157.0e3 Pa
n2=1.00

*#####
* Initialize #####
***** FBM output. Must have sufficient gas & DATA_10
* Reasonable oil content.
$INITGAS=G940 flow=1.00 mol/s temp=773 K pres=157.0e3 Pa
n2=0.613 h2=0.22 ch4=0.07 c2h4=0.037 c3h6=0.044
oil-1=0.013 oil-2=0.002 oil-3=0.001

***** Out of PYR units

$INITGAS=G1001 flow=0.064 mol/s temp=773 K pres=157.0e3 Pa
n2=0.379 h2=0.31 ch4=0.095 c2h4=0.048 c3h6=0.058
oil-1=0.033 oil-2=0.053 oil-3=0.024
$INITGAS=G1002 same_as=G1001
$INITGAS=G1003 same_as=G1001
$INITGAS=G1004 same_as=G1001

*#####
* Solids #####
*#####
* Raw Into Mixer #####
**** Total raw 2.48
$INITSOLID=RAWA temp=410 por=0.10 DATA_11
Inert=0.4249 SiO2=0.1
Kerogen-1=0.1206 CaCO3=0.2235 MgCO3=0.1310

```

```

prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.01266 kg/s   diam=0.0054  31 %
$INITOLID=RAWB same_as=RAWA   flow=0.00858 kg/s   diam=0.0035  21 %
$INITOLID=RAWC same_as=RAWA   flow=0.00898 kg/s   diam=0.0017  22 %
$INITOLID=RAWD same_as=RAWA   flow=0.00735 kg/s   diam=0.0004  18 %
$INITOLID=FRAW same_as=RAWA   flow=0.00327 kg/s   diam=0.00005 8 %

*##### Out Of Bottom Pyrolyzer (Feed to Relax & Lift) #####
***** Single Pass                                         DATA_12
$INITOLID=S1004A temp=768 por=0.17
               inert=0.4317 sio2=0.15
               mgco3=0.149 caco3=0.25 char=0.0193
prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.0100 kg/s   diam=0.0054
$INITOLID=S1004B same_as=S1004A flow=0.0070 kg/s   diam=0.0035
$INITOLID=S1004C same_as=S1004A flow=0.0070 kg/s   diam=0.0017
$INITOLID=S1004D same_as=S1004A flow=0.0065 kg/s   diam=0.0004
$INITOLID=F1004 same_as=S1004A flow=0.0025 kg/s   diam=0.00005

***** Multiple Pass                                         DATA_13
$INITOLID=M1004A temp=768 por=0.17
               inert=0.489 sio2=0.15
               MgCO3=0.06 caco3=0.25 MgO=0.04
               coke=0.005 char=0.006
prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.035 kg/s   diam=0.0047 36%
$INITOLID=M1004B temp=768 por=0.17
               inert=0.50 sio2=0.143
               MgCO3=0.06 caco3=0.25 MgO=0.04
               coke=0.005 char=0.002
prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.043 kg/s   diam=0.0030 44%
$INITOLID=M1004C temp=768 por=0.17
               inert=0.50 sio2=0.144
               MgCO3=0.06 caco3=0.25 MgO=0.04
               coke=0.005 char=0.001
prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.018 kg/s   diam=0.0015 18%
$INITOLID=M1004D temp=768 por=0.17
               inert=0.50 sio2=0.145
               MgCO3=0.06 caco3=0.25 MgO=0.04
               coke=0.005 char=0.000
prop(1)=44    kg/m**3 orig-char
prop(2)=272   kg/m**3 orig-ker
                           flow=0.002 kg/s   diam=0.0004 2%

```

OUTPUT FILE

The following is a list of selected portions of the ASCII output file for this example problem.

```
%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%
```

Title : Lab Retort H20 - 9P Sizes

Input file: h20.inp

Time : 09:02:03
Date : 30-Nov-93

Model : osp
Version: 2.0
Machine: HP-9000

%%%%%%%%%%%%%%
%%%%%%%%%%%%%

GLOBAL parameters

tol: Tolerance: .0002
loopmax: Max loops: 31
all_mod:: 0
check_con: Check Conectivity: 1
modulo_st: Modulo for stream file writes: 1
group_loop(i): Group 1 Iterations = 2

PROPERTY parameters

sphericity: Sphericity: .6000

Kinetic parameters :

	Pre-exponential	Activation	Temp
deo2_coef: 'Effective particle O2 diffusivity factor:	1.040E-15		
ns_ads: Adsorption site/m**2 (site/m**2):	1.200E+18		
solid_int: Solid internal area (m**2/m**3):	1.000E+07		
a_coke: Surface area per kg coke (m**2/kg):	1.700E+06		
coke_rfac: Coke covered area reaction factor:	.30		
del_coke: Coke defualt internal resistance length frac:	.105		
del_coke_comb: Coke default internal resistance length frac (comb):	.105		
_ker: Kerogen Pyrolysis:	2.8100E+13	26390.	
_char_comb: Char Combustion:	7.0000E+00	11080.	
_coke_comb: Coke Combustion:	1.4000E+01	11080.	
_fes2_comb: FeS2 Combustion:	1.9700E+06	20202.	
_dol(1): MgCO3 Decomp - 1:	4.0800E+07	23320.	
_dol(2): MgCO3 Decomp - 2:	9.0200E+04	17010.	
_cal(1): CaCO3 Decomp - 1:	1.3000E+10	27680.	
_cal(2): CaCO3 Decomp - 2:	5.6000E+08	29620.	
_cal(3): CaCO3 Decomp - 3:	8.5200E+12	40460.	
_pco2: CO2-Eq CaCO3 Decomp:	1.9400E+13	22360.	
_ads(1): Oil-1 Adsorption:	3.0000E-07	4730.	
_ads(2): Oil-2 Adsorption:	3.0000E-07	6730.	
_ads(3): Oil-3 Adsorption:	3.0000E-07	7730.	
_coke(1): Oil-1 Coking:	1.7000E+07	16640.	
_coke(2): Oil-2 Coking:	1.7000E+07	16640.	
_coke(3): Oil-3 Coking:	1.7000E+07	16640.	
_evap(1): Oil-1 Evap param:	1.0000E+00		
_evap(2): Oil-2 Evap param:	1.0000E-04		

_evap(3): Oil-3 Evap param: 1.0000E-04

Species parameters :

Gas	H of form. (J/mol)	Heat capacity (J/mol/K)			Viscosity (kg/m/s)		
		a	b (T)	c (T**2)	a	b (T)	
1. N2	.000E+00	2.730E+01	5.230E-03	-4.184E-09	1.730E-05	6.850E-01	
2. O2	.000E+00	2.572E+01	1.298E-02	-3.863E-06	1.730E-05	6.850E-01	
3. H2	.000E+00	2.907E+01	-8.368E-04	2.013E-06	8.300E-06	6.700E-01	
4. CO	-1.105E+05	2.686E+01	6.966E-03	-8.201E-07	1.690E-05	6.700E-01	
5. CO2	-3.935E+05	2.600E+01	4.350E-02	-1.483E-05	1.360E-05	8.700E-01	
6. H2O	-2.418E+05	3.036E+01	9.615E-03	1.184E-06	8.800E-06	1.113E+00	
7. H2S	-2.015E+04	2.787E+01	2.148E-02	-3.573E-06	3.600E-05	.000E+00	
8. SO2	-2.969E+05	2.977E+01	3.980E-02	1.469E-05	3.600E-05	.000E+00	
9. NH3	-4.619E+04	2.546E+01	3.687E-02	-6.301E-06	3.600E-05	.000E+00	
10. NO2	3.364E+04	3.000E+01	.000E+00	.000E+00	3.600E-05	.000E+00	
11. HCN	-1.300E+05	3.000E+01	.000E+00	.000E+00	3.600E-05	.000E+00	
12. COS	-9.900E+01	3.000E+01	.000E+00	.000E+00	3.600E-05	.000E+00	
13. CH4	-7.485E+04	1.415E+01	7.550E-02	-1.799E-05	1.600E-05	7.600E-01	
14. C2H4	5.228E+04	1.184E+01	1.197E-01	-3.651E-05	3.600E-05	.000E+00	
15. C2H6	-8.467E+04	9.400E+00	1.598E-01	-4.623E-05	3.600E-05	.000E+00	
16. C3H6	2.041E+04	1.361E+01	1.888E-01	-5.749E-05	3.600E-05	.000E+00	
17. C3H8	-1.039E+05	1.008E+01	2.393E-01	-7.336E-05	3.600E-05	.000E+00	
18. C5-pseudo	-8.360E+04	1.024E+01	1.885E-01	-5.866E-05	3.600E-05	.000E+00	
19. H12-pseudo	-8.360E+04	1.024E+01	1.885E-01	-5.866E-05	3.600E-05	.000E+00	
20. Oil-1	-2.690E+05	4.770E+01	7.900E-01	2.580E-04	3.600E-05	.000E+00	
21. Oil-2	-5.370E+05	1.072E+02	1.700E+00	5.500E-04	3.600E-05	.000E+00	
22. Oil-3	-7.010E+05	1.438E+02	2.250E-01	7.180E-04	3.600E-05	.000E+00	
23. Oil-4	.000E+00	6.000E+02	.000E+00	.000E+00	3.600E-05	.000E+00	
24. Oil-5	.000E+00	6.000E+02	.000E+00	.000E+00	3.600E-05	.000E+00	
25. Gas-A	.000E+00	3.000E+01	.000E+00	.000E+00	1.730E-05	6.850E-01	
26. Gas-B	.000E+00	3.000E+01	.000E+00	.000E+00	1.730E-05	6.850E-01	
27. Gas-C	.000E+00	3.000E+01	.000E+00	.000E+00	1.730E-05	6.850E-01	
28. Gas-D	.000E+00	3.000E+01	.000E+00	.000E+00	1.730E-05	6.850E-01	

Gas	C/mol	H/mol	O/mol	N/mol	S/mol	kg/mol	Dif-vol
1. N2	.00	.00	.00	2.00	.00	.0280	17.90
2. O2	.00	.00	2.00	.00	.00	.0320	16.60
3. H2	.00	2.00	.00	.00	.00	.0020	7.07
4. CO	1.00	.00	1.00	.00	.00	.0280	18.90
5. CO2	1.00	.00	2.00	.00	.00	.0440	26.90
6. H2O	.00	2.00	1.00	.00	.00	.0180	12.70
7. H2S	.00	2.00	.00	.00	1.00	.0340	21.00
8. SO2	.00	.00	2.00	.00	1.00	.0640	41.10
9. NH3	.00	3.00	.00	1.00	.00	.0170	14.90
10. NO2	.00	.00	2.00	1.00	.00	.0460	16.70
11. HCN	1.00	1.00	.00	1.00	.00	.0270	24.20
12. COS	1.00	.00	1.00	.00	1.00	.0600	39.00
13. CH4	1.00	4.00	.00	.00	.00	.0160	24.50
14. C2H4	2.00	4.00	.00	.00	.00	.0280	41.00
15. C2H6	2.00	6.00	.00	.00	.00	.0300	45.00
16. C3H6	3.00	6.00	.00	.00	.00	.0420	61.50
17. C3H8	3.00	8.00	.00	.00	.00	.0440	65.50
18. C5-pseudo	5.00	.00	.00	.00	.00	.0600	33.00
19. H12-pseudo	.00	12.00	.00	.00	.00	.0120	24.00
20. Oil-1	11.00	17.49	.22	.26	.03	.1578	228.00
21. Oil-2	24.00	38.16	.48	.57	.07	.3443	494.00
22. Oil-3	32.00	50.88	.64	.76	.10	.4590	664.00
23. Oil-4	20.00	31.20	.20	.38	.06	.2816	412.00
24. Oil-5	20.00	31.20	.20	.38	.06	.2816	412.00
25. Gas-A	.00	.00	.00	2.00	.00	.0280	17.90

26. Gas-B	.00	.00	.00	2.00	.00	.0280	17.90
27. Gas-C	.00	.00	.00	2.00	.00	.0280	17.90
28. Gas-D	.00	.00	.00	2.00	.00	.0280	17.90

Solid	H of form (J/kg)	a	Heat cap (J/kg/K)		
			b (T)	c (T**2)	d (T**-2)
1. Kerogen-1	-1.450E+06	2.130E+02	5.220E+00	-1.660E-03	.000E+00
2. Kerogen-2	.000E+00	1.500E+03	.000E+00	.000E+00	.000E+00
3. Kerogen-3	.000E+00	1.500E+03	.000E+00	.000E+00	.000E+00
4. Char-C	.000E+00	-2.670E+02	3.889E+00	-1.845E-03	.000E+00
5. Char-H	.000E+00	4.482E+03	1.707E+01	.000E+00	.000E+00
6. Char-O	.000E+00	-2.670E+02	3.889E+00	-1.845E-03	.000E+00
7. Char-N	.000E+00	-2.670E+02	3.889E+00	-1.845E-03	.000E+00
8. Char-S	.000E+00	-2.670E+02	3.889E+00	-1.845E-03	.000E+00
9. Inert	.000E+00	5.808E+02	1.262E+00	-6.468E-04	-1.270E+07
10. Moisture	-1.588E+07	4.184E+03	.000E+00	.000E+00	.000E+00
11. Bound-water	-1.614E+07	1.680E+03	2.200E+00	.000E+00	.000E+00
12. CaCO3	-1.206E+07	9.963E+02	2.690E-01	.000E+00	-2.516E+07
13. CaO	-1.133E+07	8.829E+02	1.012E-01	-1.154E-05	-1.431E+07
14. CaSO4	-1.053E+07	5.302E+02	7.150E-01	.000E+00	-1.009E+06
15. MgCO3	-1.299E+07	3.800E+02	2.029E+00	8.830E-04	.000E+00
16. MgO	-1.493E+07	1.021E+03	4.330E-01	-1.630E-04	-1.772E+07
17. MgSO4	-1.048E+07	7.524E+02	6.300E-01	-1.113E-04	1.168E+07
18. CaSiO3	-1.362E+07	2.890E+02	1.780E+00	-7.761E-04	.000E+00
19. FeS2	-1.412E+06	7.273E+02	-2.770E-01	2.579E-04	-1.326E+07
20. FeS	-1.149E+06	5.807E+02	1.133E-01	.000E+00	.000E+00
21. Fe2O3	-5.164E+06	-2.942E+02	2.805E+00	-1.542E-03	2.285E+07
22. SiO2	-1.518E+07	2.890E+02	1.780E+00	-7.761E-04	.000E+00
23. N-inorganic	.000E+00	-2.670E+02	3.889E+00	-1.845E-03	.000E+00
24. Oil-1	-1.930E+06	1.600E+03	.000E+00	.000E+00	.000E+00
25. Oil-2	-1.500E+06	1.600E+03	.000E+00	.000E+00	.000E+00
26. Oil-3	.000E+00	1.600E+03	.000E+00	.000E+00	.000E+00
27. Oil-4	.000E+00	1.600E+03	.000E+00	.000E+00	.000E+00
28. Oil-5	.000E+00	1.600E+03	.000E+00	.000E+00	.000E+00
29. Coke	.000E+00	2.130E+02	5.220E+00	-1.660E-03	.000E+00
30. Char	.000E+00	2.130E+02	5.220E+00	-1.660E-03	.000E+00
31. Solid-A	.000E+00	1.000E+03	.000E+00	.000E+00	.000E+00
32. Solid-B	.000E+00	1.000E+03	.000E+00	.000E+00	.000E+00
33. Solid-C	.000E+00	1.000E+03	.000E+00	.000E+00	.000E+00
34. Solid-D	.000E+00	1.000E+03	.000E+00	.000E+00	.000E+00

Solid	W-frac C	W-frac H	W-frac O	W-frac N	W-frac S	kg/m**3	Inorg C
1. Kerogen-1	.8374	.1047	.0223	.0244	.0112	1050.0	.0000
2. Kerogen-2	1.0000	.0000	.0000	.0000	.0000	1000.0	.0000
3. Kerogen-3	1.0000	.0000	.0000	.0000	.0000	1000.0	.0000
4. Char-C	1.0000	.0000	.0000	.0000	.0000	1050.0	.0000
5. Char-H	.0000	1.0000	.0000	.0000	.0000	1050.0	.0000
6. Char-O	.0000	.0000	1.0000	.0000	.0000	1050.0	.0000
7. Char-N	.0000	.0000	.0000	1.0000	.0000	1050.0	.0000
8. Char-S	.0000	.0000	.0000	.0000	1.0000	1050.0	.0000
9. Inert	.0000	.0000	.0000	.0000	.0000	2650.0	.0000
10. Moisture	.0000	.1111	.9000	.0000	.0000	1000.0	.0000
11. Bound-water	.0000	.1111	.9000	.0000	.0000	1000.0	.0000
12. CaCO3	.1200	.0000	.4800	.0000	.0000	2710.0	.1200
13. CaO	.0000	.0000	.2857	.0000	.0000	3350.0	.0000
14. CaSO4	.0000	.0000	.4706	.0000	.2353	2960.0	.0000
15. MgCO3	.1424	.0000	.5694	.0000	.0000	2850.0	.1424
16. MgO	.0000	.0000	.3970	.0000	.0000	3580.0	.0000
17. MgSO4	.0000	.0000	.5320	.0000	.2660	2650.0	.0000
18. CaSiO3	.0000	.0000	.4138	.0000	.0000	2650.0	.0000
19. FeS2	.0000	.0000	.0000	.0000	.5342	4980.0	.0000
20. FeS	.0000	.0000	.0000	.0000	.3645	4830.0	.0000

21. Fe2O3	.0000	.0000	.3008	.0000	.0000	5280.0	.0000
22. SiO2	.0000	.0000	.5333	.0000	.0000	2650.0	.0000
23. N-inorganic	.0000	.0000	.0000	.0000	.0000	2650.0	.0000
24. Oil-1	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
25. Oil-2	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
26. Oil-3	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
27. Oil-4	.8521	.1108	.0114	.0189	.0068	1050.0	.0000
28. Oil-5	.8521	.1108	.0114	.0189	.0068	1050.0	.0000
29. Coke	.9012	.0315	.0240	.0336	.0096	1050.0	.0000
30. Char	.8837	.0310	.0233	.0430	.0190	1050.0	.0000
31. Solid-A	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
32. Solid-B	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
33. Solid-C	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
34. Solid-D	.0000	.0000	.0000	.0000	.0000	2000.0	.0000

Liquid	H of form (J/kg)	Heat cap (J/kg/K)	a	b (T)	c (T**2)
1. Oil-1	-1.740E+06	3.079E+02	5.100E+00	1.640E-03	
2. Oil-2	-1.590E+06	3.172E+02	5.030E+00	1.630E-03	
3. Oil-3	-1.560E+06	3.191E+02	4.990E+00	1.590E-03	
4. Oil-4	-1.620E+06	3.167E+02	1.207E+00	3.835E-04	
5. Oil-5	-1.620E+06	3.167E+02	1.207E+00	3.835E-04	
6. Water	-1.588E+07	4.184E+03	.0000E+00	.0000E+00	
7. Liquid-A	.0000E+00	1.0000E+03	.0000E+00	.0000E+00	
8. Liquid-B	.0000E+00	1.0000E+03	.0000E+00	.0000E+00	

Liquid	C/molecule	H/molecule	O/molecule	N/molecule	S/molecule	kg/mol
1. Oil-1	11.0000	17.4900	.2200	.2629	.0341	.1578
2. Oil-2	24.0000	38.1600	.4800	.5736	.0744	.3443
3. Oil-3	32.0000	50.8800	.6400	.7648	.0992	.4590
4. Oil-4	20.0000	31.2000	.2000	.3800	.0600	.2816
5. Oil-5	20.0000	31.2000	.2000	.3800	.0600	.2816
6. Water	.0000	2.0000	1.0000	.0000	.0000	.0180
7. Liquid-A	.0000	2.0000	1.0000	.0000	.0000	.0180
8. Liquid-B	.0000	2.0000	1.0000	.0000	.0000	.0180

Reaction Stoichiometry:

(Note these may be overwritten by STOICH modules.)

Reactions:

- | | | |
|------------------|----------------|-----------------|
| 1. KER-1 + O2 | 2. KER-2 + O2 | 3. KER-3 + O2 |
| 4. CHAR-C + O2 | 5. CHAR-H + O2 | 6. CHAR-O + O2 |
| 7. CHAR-N + O2 | 8. CHAR-S + O2 | 9. MGCO3 DECOMP |
| 10. CACO3 DECOMP | 11. KER-1 P L | 12. KER-1 P G |
| 13. OIL-1 ADS | 14. OIL-2 ADS | 15. OIL-3 ADS |
| 16. OIL-1 COK | 17. OIL-2 COK | 18. OIL-3 COK |
| 19. COKE + O2 | 20. OIL-1 EVAP | 21. OIL-2 EVAP |
| 22. OIL-3 EVAP | 23. CHAR + O2 | 24. FES2 COMB |
| 25. CACO3 + SIO2 | 26. EXTRA 1 | 27. EXTRA 2 |
| 28. EXTRA 3 | 29. EXTRA 4 | |

Gases	Reaction					
	1	2	3	4	5	6
1. N2	.00000	.00000	.00000	.00000	.00000	.00000
2. O2	-97.35432	-83.33333	-83.33333	-83.33333-250.00000	31.25000	
3. H2	.00000	.00000	.00000	.00000	.00000	.00000
4. CO	.00000	.00000	.00000	.00000	.00000	.00000
5. CO2	69.78333	83.33333	83.33333	83.33333	.00000	.00000
6. H2O	52.35000	.00000	.00000	.00000	500.00000	.00000
7. H2S	.00000	.00000	.00000	.00000	.00000	.00000
8. SO2	.35000	.00000	.00000	.00000	.00000	.00000

9. NH3	.00000	.00000	.00000	.00000	.00000	.00000
10. NO2	1.74286	.00000	.00000	.00000	.00000	.00000
11. HCN	.00000	.00000	.00000	.00000	.00000	.00000
12. COS	.00000	.00000	.00000	.00000	.00000	.00000
13. CH4	.00000	.00000	.00000	.00000	.00000	.00000
14. C2H4	.00000	.00000	.00000	.00000	.00000	.00000
15. C2H6	.00000	.00000	.00000	.00000	.00000	.00000
16. C3H6	.00000	.00000	.00000	.00000	.00000	.00000
17. C3H8	.00000	.00000	.00000	.00000	.00000	.00000
18. C5-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
19. H12-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
20. Oil-1	.00000	.00000	.00000	.00000	.00000	.00000
21. Oil-2	.00000	.00000	.00000	.00000	.00000	.00000
22. Oil-3	.00000	.00000	.00000	.00000	.00000	.00000
23. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
25. Gas-A	.00000	.00000	.00000	.00000	.00000	.00000
26. Gas-B	.00000	.00000	.00000	.00000	.00000	.00000
27. Gas-C	.00000	.00000	.00000	.00000	.00000	.00000
28. Gas-D	.00000	.00000	.00000	.00000	.00000	.00000
Solids						
1. Kerogen-1	-1.00000	.00000	.00000	.00000	.00000	.00000
2. Kerogen-2	.00000	-1.00000	.00000	.00000	.00000	.00000
3. Kerogen-3	.00000	.00000	-1.00000	.00000	.00000	.00000
4. Char-C	.00000	.00000	.00000	-1.00000	.00000	.00000
5. Char-H	.00000	.00000	.00000	.00000	-1.00000	.00000
6. Char-O	.00000	.00000	.00000	.00000	.00000	-1.00000
7. Char-N	.00000	.00000	.00000	.00000	.00000	.00000
8. Char-S	.00000	.00000	.00000	.00000	.00000	.00000
9. Inert	.00000	.00000	.00000	.00000	.00000	.00000
10. Moisture	.00000	.00000	.00000	.00000	.00000	.00000
11. Bound-water	.00000	.00000	.00000	.00000	.00000	.00000
12. CaCO3	.00000	.00000	.00000	.00000	.00000	.00000
13. CaO	.00000	.00000	.00000	.00000	.00000	.00000
14. CaSO4	.00000	.00000	.00000	.00000	.00000	.00000
15. MgCO3	.00000	.00000	.00000	.00000	.00000	.00000
16. MgO	.00000	.00000	.00000	.00000	.00000	.00000
17. MgSO4	.00000	.00000	.00000	.00000	.00000	.00000
18. CaSiO3	.00000	.00000	.00000	.00000	.00000	.00000
19. FeS2	.00000	.00000	.00000	.00000	.00000	.00000
20. FeS	.00000	.00000	.00000	.00000	.00000	.00000
21. Fe2O3	.00000	.00000	.00000	.00000	.00000	.00000
22. SiO2	.00000	.00000	.00000	.00000	.00000	.00000
23. N-inorganic	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-1	.00000	.00000	.00000	.00000	.00000	.00000
25. Oil-2	.00000	.00000	.00000	.00000	.00000	.00000
26. Oil-3	.00000	.00000	.00000	.00000	.00000	.00000
27. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
28. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
29. Coke	.00000	.00000	.00000	.00000	.00000	.00000
30. Char	.00000	.00000	.00000	.00000	.00000	.00000
31. Solid-A	.00000	.00000	.00000	.00000	.00000	.00000
32. Solid-B	.00000	.00000	.00000	.00000	.00000	.00000
33. Solid-C	.00000	.00000	.00000	.00000	.00000	.00000
34. Solid-D	.00000	.00000	.00000	.00000	.00000	.00000
Liquids						
1. Oil-1	.00000	.00000	.00000	.00000	.00000	.00000
2. Oil-2	.00000	.00000	.00000	.00000	.00000	.00000
3. Oil-3	.00000	.00000	.00000	.00000	.00000	.00000
4. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
5. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
6. Water	.00000	.00000	.00000	.00000	.00000	.00000
7. Liquid-A	.00000	.00000	.00000	.00000	.00000	.00000
8. Liquid-B	.00000	.00000	.00000	.00000	.00000	.00000

		Reaction					
Gases		7	8	9	10	11	12
1. N2		.00000	.00000	.00000	.00000	.00000	.00000
2. O2		-71.42857	-31.25000	.00000	.00000	.00000	.00000
3. H2		.00000	.00000	.00000	.00000	1.65909	1.65909
4. CO		.00000	.00000	.00000	.00000	.00000	.00000
5. CO2		.00000	.00000	11.86240	10.00000	.00000	.00000
6. H2O		.00000	.00000	.00000	.00000	.11835	.11835
7. H2S		.00000	.00000	.00000	.00000	.09225	.09225
8. SO2		.00000	31.25000	.00000	.00000	.00000	.00000
9. NH3		.00000	.00000	.00000	.00000	.00256	.00256
10. NO2		71.42857	.00000	.00000	.00000	.00000	.00000
11. HCN		.00000	.00000	.00000	.00000	.00000	.00000
12. COS		.00000	.00000	.00000	.00000	.00000	.00000
13. CH4		.00000	.00000	.00000	.00000	.80000	.80000
14. C2H4		.00000	.00000	.00000	.00000	.56000	.56000
15. C2H6		.00000	.00000	.00000	.00000	.00000	.00000
16. C3H6		.00000	.00000	.00000	.00000	1.32659	1.32659
17. C3H8		.00000	.00000	.00000	.00000	.00000	.00000
18. C5-pseudo		.00000	.00000	.00000	.00000	.00000	.00000
19. H12-pseudo		.00000	.00000	.00000	.00000	.00000	.00000
20. Oil-1		.00000	.00000	.00000	.00000	.00000	2.35887
21. Oil-2		.00000	.00000	.00000	.00000	.00000	.54058
22. Oil-3		.00000	.00000	.00000	.00000	.00000	.40543
23. Oil-4		.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-5		.00000	.00000	.00000	.00000	.00000	.00000
25. Gas-A		.00000	.00000	.00000	.00000	.00000	.00000
26. Gas-B		.00000	.00000	.00000	.00000	.00000	.00000
27. Gas-C		.00000	.00000	.00000	.00000	.00000	.00000
28. Gas-D		.00000	.00000	.00000	.00000	.00000	.00000
Solids							
1. Kerogen-1		.00000	.00000	.00000	.00000	-1.00000	-1.00000
2. Kerogen-2		.00000	.00000	.00000	.00000	.00000	.00000
3. Kerogen-3		.00000	.00000	.00000	.00000	.00000	.00000
4. Char-C		.00000	.00000	.00000	.00000	.00000	.00000
5. Char-H		.00000	.00000	.00000	.00000	.00000	.00000
6. Char-O		.00000	.00000	.00000	.00000	.00000	.00000
7. Char-N		-1.00000	.00000	.00000	.00000	.00000	.00000
8. Char-S		.00000	-1.00000	.00000	.00000	.00000	.00000
9. Inert		.00000	.00000	.00000	.00000	.00000	.00000
10. Moisture		.00000	.00000	.00000	.00000	.00000	.00000
11. Bound-water		.00000	.00000	.00000	.00000	.00000	.00000
12. CaCO3		.00000	.00000	.00000	-1.00000	.00000	.00000
13. CaO		.00000	.00000	.00000	.56001	.00000	.00000
14. CaSO4		.00000	.00000	.00000	.00000	.00000	.00000
15. MgCO3		.00000	.00000	-1.00000	.00000	.00000	.00000
16. MgO		.00000	.00000	.47806	.00000	.00000	.00000
17. MgSO4		.00000	.00000	.00000	.00000	.00000	.00000
18. CaSiO3		.00000	.00000	.00000	.00000	.00000	.00000
19. FeS2		.00000	.00000	.00000	.00000	.00000	.00000
20. FeS		.00000	.00000	.00000	.00000	.00000	.00000
21. Fe2O3		.00000	.00000	.00000	.00000	.00000	.00000
22. SiO2		.00000	.00000	.00000	.00000	.00000	.00000
23. N-inorganic		.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-1		.00000	.00000	.00000	.00000	.00000	.00000
25. Oil-2		.00000	.00000	.00000	.00000	.00000	.00000
26. Oil-3		.00000	.00000	.00000	.00000	.00000	.00000
27. Oil-4		.00000	.00000	.00000	.00000	.00000	.00000
28. Oil-5		.00000	.00000	.00000	.00000	.00000	.00000
29. Coke		.00000	.00000	.00000	.00000	.00000	.00000
30. Char		.00000	.00000	.00000	.00000	.16280	.16280
31. Solid-A		.00000	.00000	.00000	.00000	.00000	.00000
32. Solid-B		.00000	.00000	.00000	.00000	.00000	.00000

33. Solid-C	.00000	.00000	.00000	.00000	.00000	.00000
34. Solid-D	.00000	.00000	.00000	.00000	.00000	.00000
Liquids						
1. Oil-1	.00000	.00000	.00000	.00000	.37219	.00000
2. Oil-2	.00000	.00000	.00000	.00000	.18609	.00000
3. Oil-3	.00000	.00000	.00000	.00000	.18609	.00000
4. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
5. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
6. Water	.00000	.00000	.00000	.00000	.00000	.00000
7. Liquid-A	.00000	.00000	.00000	.00000	.00000	.00000
8. Liquid-B	.00000	.00000	.00000	.00000	.00000	.00000

Gases	Reaction					
	13	14	15	16	17	18
1. N2	.00000	.00000	.00000	.00000	.00000	.00000
2. O2	.00000	.00000	.00000	.00000	.00000	.00000
3. H2	.00000	.00000	.00000	21.03320	21.03320	21.03320
4. CO	.00000	.00000	.00000	.00000	.00000	.00000
5. CO2	.00000	.00000	.00000	.14188	.14188	.14188
6. H2O	.00000	.00000	.00000	.09000	.09000	.09000
7. H2S	.00000	.00000	.00000	.01163	.01163	.01163
8. SO2	.00000	.00000	.00000	.00000	.00000	.00000
9. NH3	.00000	.00000	.00000	.03229	.03229	.03229
10. NO2	.00000	.00000	.00000	.00000	.00000	.00000
11. HCN	.00000	.00000	.00000	.00000	.00000	.00000
12. COS	.00000	.00000	.00000	.00000	.00000	.00000
13. CH4	.00000	.00000	.00000	5.00000	5.00000	5.00000
14. C2H4	.00000	.00000	.00000	3.50000	3.50000	3.50000
15. C2H6	.00000	.00000	.00000	.00000	.00000	.00000
16. C3H6	.00000	.00000	.00000	2.16893	2.16893	2.16893
17. C3H8	.00000	.00000	.00000	.00000	.00000	.00000
18. C5-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
19. H12-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
20. Oil-1	-1.00000	.00000	.00000	.00000	.00000	.00000
21. Oil-2	.00000	-1.00000	.00000	.00000	.00000	.00000
22. Oil-3	.00000	.00000	-1.00000	.00000	.00000	.00000
23. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
25. Gas-A	.00000	.00000	.00000	.00000	.00000	.00000
26. Gas-B	.00000	.00000	.00000	.00000	.00000	.00000
27. Gas-C	.00000	.00000	.00000	.00000	.00000	.00000
28. Gas-D	.00000	.00000	.00000	.00000	.00000	.00000
Solids						
1. Kerogen-1	.00000	.00000	.00000	.00000	.00000	.00000
2. Kerogen-2	.00000	.00000	.00000	.00000	.00000	.00000
3. Kerogen-3	.00000	.00000	.00000	.00000	.00000	.00000
4. Char-C	.00000	.00000	.00000	.00000	.00000	.00000
5. Char-H	.00000	.00000	.00000	.00000	.00000	.00000
6. Char-O	.00000	.00000	.00000	.00000	.00000	.00000
7. Char-N	.00000	.00000	.00000	.00000	.00000	.00000
8. Char-S	.00000	.00000	.00000	.00000	.00000	.00000
9. Inert	.00000	.00000	.00000	.00000	.00000	.00000
10. Moisture	.00000	.00000	.00000	.00000	.00000	.00000
11. Bound-water	.00000	.00000	.00000	.00000	.00000	.00000
12. CaCO3	.00000	.00000	.00000	.00000	.00000	.00000
13. CaO	.00000	.00000	.00000	.00000	.00000	.00000
14. CaSO4	.00000	.00000	.00000	.00000	.00000	.00000
15. MgCO3	.00000	.00000	.00000	.00000	.00000	.00000
16. MgO	.00000	.00000	.00000	.00000	.00000	.00000
17. MgSO4	.00000	.00000	.00000	.00000	.00000	.00000
18. CaSiO3	.00000	.00000	.00000	.00000	.00000	.00000
19. FeS2	.00000	.00000	.00000	.00000	.00000	.00000
20. FeS	.00000	.00000	.00000	.00000	.00000	.00000
21. Fe2O3	.00000	.00000	.00000	.00000	.00000	.00000

22. SiO2	.00000	.00000	.00000	.00000	.00000	.00000
23. N-inorganic	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-1	.15778	.00000	.00000	-1.00000	.00000	.00000
25. Oil-2	.00000	.34425	.00000	.00000	-1.00000	.00000
26. Oil-3	.00000	.00000	.45900	.00000	.00000	-1.00000
27. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
28. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
29. Coke	.00000	.00000	.00000	.68000	.68000	.68000
30. Char	.00000	.00000	.00000	.00000	.00000	.00000
31. Solid-A	.00000	.00000	.00000	.00000	.00000	.00000
32. Solid-B	.00000	.00000	.00000	.00000	.00000	.00000
33. Solid-C	.00000	.00000	.00000	.00000	.00000	.00000
34. Solid-D	.00000	.00000	.00000	.00000	.00000	.00000
Liquids						
1. Oil-1	.00000	.00000	.00000	.00000	.00000	.00000
2. Oil-2	.00000	.00000	.00000	.00000	.00000	.00000
3. Oil-3	.00000	.00000	.00000	.00000	.00000	.00000
4. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
5. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
6. Water	.00000	.00000	.00000	.00000	.00000	.00000
7. Liquid-A	.00000	.00000	.00000	.00000	.00000	.00000
8. Liquid-B	.00000	.00000	.00000	.00000	.00000	.00000

Gases	Reaction					
	19	20	21	22	23	24
1. N2	.00000	.00000	.00000	.00000	.00000	.00000
2. O2	-84.92500	.00000	.00000	.00000	-84.31872	-31.30220
3. H2	.00000	.00000	.00000	.00000	.00000	.00000
4. CO	.00000	.00000	.00000	.00000	.00000	.00000
5. CO2	75.10000	.00000	.00000	.00000	73.64167	16.69450
6. H2O	15.75000	.00000	.00000	.00000	15.48000	.00000
7. H2S	.00000	.00000	.00000	.00000	.00000	.00000
8. SO2	.30000	.00000	.00000	.00000	.59500	.00000
9. NH3	.00000	.00000	.00000	.00000	.00000	.00000
10. NO2	2.40000	.00000	.00000	.00000	3.07143	.00000
11. HCN	.00000	.00000	.00000	.00000	.00000	.00000
12. COS	.00000	.00000	.00000	.00000	.00000	.00000
13. CH4	.00000	.00000	.00000	.00000	.00000	.00000
14. C2H4	.00000	.00000	.00000	.00000	.00000	.00000
15. C2H6	.00000	.00000	.00000	.00000	.00000	.00000
16. C3H6	.00000	.00000	.00000	.00000	.00000	.00000
17. C3H8	.00000	.00000	.00000	.00000	.00000	.00000
18. C5-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
19. H12-pseudo	.00000	.00000	.00000	.00000	.00000	.00000
20. Oil-1	.00000	6.33787	.00000	.00000	.00000	.00000
21. Oil-2	.00000	.00000	2.90486	.00000	.00000	.00000
22. Oil-3	.00000	.00000	.00000	2.17864	.00000	.00000
23. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
25. Gas-A	.00000	.00000	.00000	.00000	.00000	.00000
26. Gas-B	.00000	.00000	.00000	.00000	.00000	.00000
27. Gas-C	.00000	.00000	.00000	.00000	.00000	.00000
28. Gas-D	.00000	.00000	.00000	.00000	.00000	.00000
Solids						
1. Kerogen-1	.00000	.00000	.00000	.00000	.00000	.00000
2. Kerogen-2	.00000	.00000	.00000	.00000	.00000	.00000
3. Kerogen-3	.00000	.00000	.00000	.00000	.00000	.00000
4. Char-C	.00000	.00000	.00000	.00000	.00000	.00000
5. Char-H	.00000	.00000	.00000	.00000	.00000	.00000
6. Char-O	.00000	.00000	.00000	.00000	.00000	.00000
7. Char-N	.00000	.00000	.00000	.00000	.00000	.00000
8. Char-S	.00000	.00000	.00000	.00000	.00000	.00000
9. Inert	.00000	.00000	.00000	.00000	.00000	.00000
10. Moisture	.00000	.00000	.00000	.00000	.00000	.00000

11. Bound-water	.00000	.00000	.00000	.00000	.00000	.00000
12. CaCO3	.00000	.00000	.00000	.00000	.00000	-1.66945
13. CaO	.00000	.00000	.00000	.00000	.00000	.00000
14. CaSO4	.00000	.00000	.00000	.00000	.00000	2.27044
15. MgCO3	.00000	.00000	.00000	.00000	.00000	.00000
16. MgO	.00000	.00000	.00000	.00000	.00000	.00000
17. MgSO4	.00000	.00000	.00000	.00000	.00000	.00000
18. CaSiO3	.00000	.00000	.00000	.00000	.00000	.00000
19. FeS2	.00000	.00000	.00000	.00000	.00000	-1.00000
20. FeS	.00000	.00000	.00000	.00000	.00000	.00000
21. Fe2O3	.00000	.00000	.00000	.00000	.00000	.66613
22. SiO2	.00000	.00000	.00000	.00000	.00000	.00000
23. N-inorganic	.00000	.00000	.00000	.00000	.00000	.00000
24. Oil-1	.00000	.00000	.00000	.00000	.00000	.00000
25. Oil-2	.00000	.00000	.00000	.00000	.00000	.00000
26. Oil-3	.00000	.00000	.00000	.00000	.00000	.00000
27. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
28. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
29. Coke	-1.00000	.00000	.00000	.00000	.00000	.00000
30. Char	.00000	.00000	.00000	.00000	-1.00000	.00000
31. Solid-A	.00000	.00000	.00000	.00000	.00000	.00000
32. Solid-B	.00000	.00000	.00000	.00000	.00000	.00000
33. Solid-C	.00000	.00000	.00000	.00000	.00000	.00000
34. Solid-D	.00000	.00000	.00000	.00000	.00000	.00000
Liquids						
1. Oil-1	.00000	-1.00000	.00000	.00000	.00000	.00000
2. Oil-2	.00000	.00000	-1.00000	.00000	.00000	.00000
3. Oil-3	.00000	.00000	.00000	-1.00000	.00000	.00000
4. Oil-4	.00000	.00000	.00000	.00000	.00000	.00000
5. Oil-5	.00000	.00000	.00000	.00000	.00000	.00000
6. Water	.00000	.00000	.00000	.00000	.00000	.00000
7. Liquid-A	.00000	.00000	.00000	.00000	.00000	.00000
8. Liquid-B	.00000	.00000	.00000	.00000	.00000	.00000

----- Reaction -----					
Gases	25	26	27	28	29
1. N2	.00000	.00000	.00000	.00000	.00000
2. O2	.00000	.00000	.00000	.00000	.00000
3. H2	.00000	.00000	.00000	.00000	.00000
4. CO	.00000	.00000	.00000	.00000	.00000
5. CO2	10.00000	.00000	.00000	.00000	.00000
6. H2O	.00000	.00000	.00000	.00000	.00000
7. H2S	.00000	.00000	.00000	.00000	.00000
8. SO2	.00000	.00000	.00000	.00000	.00000
9. NH3	.00000	.00000	.00000	.00000	.00000
10. NO2	.00000	.00000	.00000	.00000	.00000
11. HCN	.00000	.00000	.00000	.00000	.00000
12. COS	.00000	.00000	.00000	.00000	.00000
13. CH4	.00000	.00000	.00000	.00000	.00000
14. C2H4	.00000	.00000	.00000	.00000	.00000
15. C2H6	.00000	.00000	.00000	.00000	.00000
16. C3H6	.00000	.00000	.00000	.00000	.00000
17. C3H8	.00000	.00000	.00000	.00000	.00000
18. C5-pseudo	.00000	.00000	.00000	.00000	.00000
19. H12-pseudo	.00000	.00000	.00000	.00000	.00000
20. Oil-1	.00000	.00000	.00000	.00000	.00000
21. Oil-2	.00000	.00000	.00000	.00000	.00000
22. Oil-3	.00000	.00000	.00000	.00000	.00000
23. Oil-4	.00000	.00000	.00000	.00000	.00000
24. Oil-5	.00000	.00000	.00000	.00000	.00000
25. Gas-A	.00000	.00000	.00000	.00000	.00000
26. Gas-B	.00000	.00000	.00000	.00000	.00000
27. Gas-C	.00000	.00000	.00000	.00000	.00000
28. Gas-D	.00000	.00000	.00000	.00000	.00000

Solids					
1. Kerogen-1	.00000	.00000	.00000	.00000	.00000
2. Kerogen-2	.00000	.00000	.00000	.00000	.00000
3. Kerogen-3	.00000	.00000	.00000	.00000	.00000
4. Char-C	.00000	.00000	.00000	.00000	.00000
5. Char-H	.00000	.00000	.00000	.00000	.00000
6. Char-O	.00000	.00000	.00000	.00000	.00000
7. Char-N	.00000	.00000	.00000	.00000	.00000
8. Char-S	.00000	.00000	.00000	.00000	.00000
9. Inert	.00000	.00000	.00000	.00000	.00000
10. Moisture	.00000	.00000	.00000	.00000	.00000
11. Bound-water	.00000	.00000	.00000	.00000	.00000
12. CaCO ₃	-1.00000	.00000	.00000	.00000	.00000
13. CaO	.00000	.00000	.00000	.00000	.00000
14. CaSO ₄	.00000	.00000	.00000	.00000	.00000
15. MgCO ₃	.00000	.00000	.00000	.00000	.00000
16. MgO	.00000	.00000	.00000	.00000	.00000
17. MgSO ₄	.00000	.00000	.00000	.00000	.00000
18. CaSiO ₃	1.16000	.00000	.00000	.00000	.00000
19. FeS ₂	.00000	.00000	.00000	.00000	.00000
20. FeS	.00000	.00000	.00000	.00000	.00000
21. Fe ₂ O ₃	.00000	.00000	.00000	.00000	.00000
22. SiO ₂	-.60000	.00000	.00000	.00000	.00000
23. N-inorganic	.00000	.00000	.00000	.00000	.00000
24. Oil-1	.00000	.00000	.00000	.00000	.00000
25. Oil-2	.00000	.00000	.00000	.00000	.00000
26. Oil-3	.00000	.00000	.00000	.00000	.00000
27. Oil-4	.00000	.00000	.00000	.00000	.00000
28. Oil-5	.00000	.00000	.00000	.00000	.00000
29. Coke	.00000	.00000	.00000	.00000	.00000
30. Char	.00000	.00000	.00000	.00000	.00000
31. Solid-A	.00000	.00000	.00000	.00000	.00000
32. Solid-B	.00000	.00000	.00000	.00000	.00000
33. Solid-C	.00000	.00000	.00000	.00000	.00000
34. Solid-D	.00000	.00000	.00000	.00000	.00000
Liquids					
1. Oil-1	.00000	.00000	.00000	.00000	.00000
2. Oil-2	.00000	.00000	.00000	.00000	.00000
3. Oil-3	.00000	.00000	.00000	.00000	.00000
4. Oil-4	.00000	.00000	.00000	.00000	.00000
5. Oil-5	.00000	.00000	.00000	.00000	.00000
6. Water	.00000	.00000	.00000	.00000	.00000
7. Liquid-A	.00000	.00000	.00000	.00000	.00000
8. Liquid-B	.00000	.00000	.00000	.00000	.00000

L

Module 8 : LIFT_PIPE Lift Pipe
Tag : 201 Group : 0 Version : 1.1

Stream connections:

GI =LFT_GIN	GO =G201	SI =S111A	SI =S112B
SI =S113C	SI =S114D	SI =M101A	SI =M101B
SI =M101C	SI =M101D	SI =F120	SO =S201A
SO =S201B	SO =S201C	SO =S201D	SO =M201A
SO =M201B	SO =M201C	SO =M201D	SO =F201

Gases	Solids	1p	2p	3p	4p	5p	6p	7p	8p	9p	Liquids
-------	--------	----	----	----	----	----	----	----	----	----	---------

Temp.	1	Temp.	17	31	45	59	73	87	101	115	129
Pres.											
N2	2	Kerogen-1	18	32	46	60	74	88	102	116	130
O2	3	Kerogen-2									
H2	4	Kerogen-3									
CO		Char-C									
CO2	5	Char-H									
H2O	6	Char-O									
H2S	7	Char-N									
SO2	8	Char-S									
NH3	9	Inert	19	33	47	61	75	89	103	117	131
NO2	10	Moisture									
HCN		Bound-water									
COS		CaCO3	20	34	48	62	76	90	104	118	132
CH4	11	CaO	21	35	49	63	77	91	105	119	133
C2H4	12	CaSO4									
C2H6		MgCO3	22	36	50	64	78	92	106	120	134
C3H6	13	MgO	23	37	51	65	79	93	107	121	135
C3H8		MgSO4									
C5-pseudo		CaSiO3	24	38	52	66	80	94	108	122	136
H12-pseudo		FeS2									
Oil-1	14	FeS									
Oil-2	15	Fe2O3									
Oil-3	16	SiO2	25	39	53	67	81	95	109	123	137
Oil-4		N-inorganic									
Oil-5		Oil-1	26	40	54	68	82	96	110	124	138
Gas-A		Oil-2	27	41	55	69	83	97	111	125	139
Gas-B		Oil-3	28	42	56	70	84	98	112	126	140
Gas-C		Oil-4									
Gas-D		Oil-5									
		Coke	29	43	57	71	85	99	113	127	141
		Char	30	44	58	72	86	100	114	128	142
		Solid-A									
		Solid-B									
		Solid-C									
		Solid-D									

Reactions:

1. KER-1 + O2	9. MGC03 DECOMP	10. CACO3 DECOMP
16. OIL-1 COK	17. OIL-2 COK	18. OIL-3 COK
19. COKE + O2	23. CHAR + O2	25. CACO3 + SIO2

ns_ads: Adsorption sites (sites/m**2) : 1.200E+18
del_coke: Coking parameter : 1.050E-01
del_coke: Coke combustion parameter : 2.000E-02
dil_mv: Diluent molecular volume : 1.790E+01
dil_mw: Diluent molecular weight : 2.800E-02
pran: Gas Prandtl number : 7.000E-01
diam: Reactor diameter (m) : .0570
height: Reactor height (m) : 9.2000
ibed:: 1
idilute:: 1
emissivity:: .00
h_loss:: .00
t_ambient:: .00
vslipcalc:: 1
icycmaxin:: 10000
dtin:: .00010
cwin:: .03000
anuin:: 2.00000

L

Stream Maps:

Solids:

[1] RAWA	[2] RAWB	[3] RAWC	[4] RAWD	[5] FRAW
[6] S1004A	[7] S1004B	[8] S1004C	[9] S1004D	[10] F1004
[11] M1004A	[12] M1004B	[13] M1004C	[14] M1004D	[15] S101A
[16] S101B	[17] S101C	[18] S101D	[19] M101A	[20] M101B
[21] M101C	[22] M101D	[23] F101	[24] S102A	[25] S102B
[26] S102C	[27] S102D	[28] F102	[29] S111A	[30] F111
[31] S112B	[32] F112	[33] S113C	[34] F113	[35] S114D
[36] F114	[37] F120	[38] S201A	[39] S201B	[40] S201C
[41] S201D	[42] M201A	[43] M201B	[44] M201C	[45] M201D
[46] F201	[47] S301A	[48] F301	[49] S302B	[50] F302
[51] S303C	[52] F303	[53] S304D	[54] F304	[55] M321A
[56] F321	[57] M322B	[58] F322	[59] M323C	[60] F323
[61] M324D	[62] F324	[63] F330	[64] F310	[65] S401A
[66] S401B	[67] S401C	[68] S401D	[69] M401A	[70] M401B
[71] M401C	[72] M401D	[73] F401	[74] DFC_FOUT	[75] S501A
[76] S501B	[77] S501C	[78] S502B	[79] S502C	[80] S502D
[81] S503C	[82] S503D	[83] S512B	[84] S513C	[85] S514D
[86] M521A	[87] M521B	[88] M521C	[89] M522B	[90] M522C
[91] M522D	[92] M523C	[93] M523D	[94] M532B	[95] M533C
[96] M534D	[97] S601A	[98] S601B	[99] S601C	[100] S601D
[101] M601A	[102] M601B	[103] M601C	[104] M601D	[105] S611A
[106] SA_SOUT	[107] M611A	[108] MA_SOUT	[109] S612B	[110] SB_SOUT
[111] M612B	[112] MB_SOUT	[113] S613C	[114] SC_SOUT	[115] M613C
[116] MC_SOUT	[117] S614D	[118] SD_SOUT	[119] M614D	[120] MD_SOUT
[121] S621A	[122] S621B	[123] S621C	[124] S621D	[125] M621A
[126] M621B	[127] M621C	[128] M621D	[129] M711A	[130] M712B
[131] M713C	[132] M714D	[133] S913A	[134] S913B	[135] S913C
[136] S913D	[137] M913A	[138] M913B	[139] M913C	[140] M913D
[141] S912A	[142] S912B	[143] S912C	[144] S912D	[145] M912A
[146] M912B	[147] M912C	[148] M912D	[149] S911A	[150] S911B
[151] S911C	[152] S911D	[153] M911A	[154] M911B	[155] M911C
[156] M911D	[157] S921A	[158] S921B	[159] S921C	[160] S921D
[161] M921A	[162] M921B	[163] M921C	[164] M921D	[165] S922A
[166] S922B	[167] S922C	[168] S922D	[169] M922A	[170] M922B
[171] M922C	[172] M922D	[173] S923A	[174] S923B	[175] S923C
[176] S923D	[177] M923A	[178] M923B	[179] M923C	[180] M923D
[181] F940	[182] S1001A	[183] S1001B	[184] S1001C	[185] S1001D
[186] M1001A	[187] M1001B	[188] M1001C	[189] M1001D	[190] F1001
[191] S1002A	[192] S1002B	[193] S1002C	[194] S1002D	[195] M1002A
[196] M1002B	[197] M1002C	[198] M1002D	[199] F1002	[200] S1003A
[201] S1003B	[202] S1003C	[203] S1003D	[204] M1003A	[205] M1003B
[206] M1003C	[207] M1003D	[208] F1003		

Gases:

[1] LFT_GIN	[2] FBC_GIN	[3] GN2MAKE	[4] CL_GIN	[5] G940
[6] G1001	[7] G1002	[8] G1003	[9] G1004	[10] G201
[11] G401	[12] DFC_GOUT	[13] G630	[14] FBC_GOUT	[15] G621
[16] CL_GOUT	[17] G801	[18] G802	[19] G810	[20] 1G820
[21] 2G820	[22] G822	[23] G823	[24] G821	[25] PYR_GOUT
[26] G824	[27] 1G901	[28] 2G901	[29] G912	[30] G913
[31] B 55 1	[32] G911	[33] B 56 1	[34] B 57 1	[35] G921
[36] B 58 1	[37] G922	[38] B 59 1	[39] G923	[40] B 60 1
[41] G930	[42] 1G1011	[43] 2G1011	[44] 1G1012	[45] 2G1012
[46] 1G1013	[47] 2G1013			

Liquids:

```
[ 1] 1_LOUT      [ 2] 2L810      [ 3] 3L810      [ 4] L811      [ 5] L812
[ 6] 2&3_LOUT    [ 7] LDUM
```

Internal stream numbers not used in any module:

```
Solids : ( 208 mapped)
209 210 211 212 213 214 215 216 217 218
219 220 221 222 223 224 225 226 227 228
229 230 231 232 233 234 235 236 237 238
239 240 241 242 243 244 245 246 247 248
249 250 251 252 253 254 255 256 257 258
259 260 261 262 263 264 265 266 267 268
269 270 271 272 273 274 275 276 277 278
279 280 281 282 283 284 285 286 287 288
289 290 291 292 293 294 295 296 297 298
299 300 301 302 303 304 305 306 307 308
309 310 311 312 313 314 315 316 317 318
319 320 321 322 323 324 325 326 327 328
329 330 331 332 333 334 335 336 337 338
339 340 341 342 343 344 345 346 347 348
349 350 351 352 353 354 355 356 357 358
359 360 361 362 363 364 365 366 367 368
369 370 371 372 373 374 375 376 377 378
379 380 381 382 383 384 385 386 387 388
389 390 391 392 393 394 395 396 397 398
399 400

Gases : ( 47 mapped)
48  49  50   51  52  53  54  55  56  57
58  59  60   61  62  63  64  65  66  67
68  69  70   71  72  73  74  75  76  77
78  79  80   81  82  83  84  85  86  87
88  89  90   91  92  93  94  95  96  97
98  99  100

Liquids: (  7 mapped)
8   9   10
```

Connection problems:

```
Possible problem: Gas stream LFT_GIN more INs than OUTs, net INs= 1
Possible problem: Gas stream FBC_GIN more INs than OUTs, net INs= 1
Possible problem: Gas stream GN2MAKE more INs than OUTs, net INs= 1
Possible problem: Gas stream CL_GIN more INs than OUTs, net INs= 4
Possible problem: Gas stream DFC_GOUT more OUTs than INs, net OUTs= 1
Possible problem: Gas stream FBC_GOUT more OUTs than INs, net OUTs= 1
Possible problem: Gas stream CL_GOUT more OUTs than INs, net OUTs= 4
Possible problem: Gas stream PYR_GOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream RAWA more INs than OUTs, net INs= 1
Possible problem: Solid stream RAWB more INs than OUTs, net INs= 1
Possible problem: Solid stream RAWC more INs than OUTs, net INs= 1
Possible problem: Solid stream RAWD more INs than OUTs, net INs= 1
Possible problem: Solid stream FRAW more INs than OUTs, net INs= 1
Possible problem: Solid stream DFC_FOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream SA_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream MA_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream SB_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream MB_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream SC_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream MC_SOUT more OUTs than INs, net OUTs= 1
Possible problem: Solid stream SD_SOUT more OUTs than INs, net OUTs= 1
```

Possible problem: Solid stream MD_SOUT more OUTs than INs, net OUTs= 1
 Possible problem: Liquid stream 1_LOUT more OUTs than INs, net OUTs= 1
 Possible problem: Liquid stream 2&3_LOUT more OUTs than INs, net OUTs= 1
 Possible problem: Liquid stream LDUM more OUTs than INs, net OUTs= 1

Loop = 1	Run time (mins) = 14.10		
101 PASS_THRU	102 RELAX	111 ATTRITION	112 ATTRITION
.00000	.76800	.00000	.00000
113 ATTRITION	114 ATTRITION	120 MERGE_STRMS	201 LIFT_PIPE
.00000	.00000	.76800	.83585
301 ATTRITION	302 ATTRITION	303 ATTRITION	304 ATTRITION
.00000	.00000	.00000	.00000
321 ATTRITION	322 ATTRITION	323 ATTRITION	324 ATTRITION
.00000	.00000	.00000	.00000
330 MERGE_STRMS	310 MERGE_STRMS	401 CO_CURRENT	402 LIFT_PIPE
.83288	.83178	.92248	.95197
501 ATTRITION	502 ATTRITION	503 ATTRITION	512 MERGE_STRMS
.00000	.00000	.00000	.93858
513 MERGE_STRMS	514 MERGE_STRMS	521 ATTRITION	522 ATTRITION
.94196	.92932	.00000	.00000
523 ATTRITION	532 MERGE_STRMS	533 MERGE_STRMS	534 MERGE_STRMS
.00000	.91592	.91634	.91919
601 CSTR	611 SPLIT_STRMS	612 SPLIT_STRMS	613 SPLIT_STRMS
.00000	.00000	.00000	.00000
614 SPLIT_STRMS	621 CSTR	630 MERGE_STRMS	711 MERGE_STRMS
.00000	.00000	.96360	1.93999
712 MERGE_STRMS	713 MERGE_STRMS	714 MERGE_STRMS	801 MERGE_STRMS
.96999	.97000	.97000	.77300
802 MERGE_STRMS	810 PHASE_CHANGE	811 MERGE_STRMS	812 SPLIT_STRMS
.77300	.00000	.41500	.00000
820 SPLIT_STRMS	822 MERGE_STRMS	823 PHASE_CHANGE	821 SPLIT_STRMS
.00000	.44214	.00000	.00000
824 PHASE_CHANGE	901 SPLIT_STRMS	913 FLUID_BED	912 FLUID_BED
.00000	.00000	.77285	.79037
911 FLUID_BED	921 FLUID_BED	922 FLUID_BED	923 FLUID_BED
.79319	.79220	.79187	.79140
930 MERGE_STRMS	940 CNTR_CURRENT	1011 SPLIT_STRMS	1012 SPLIT_STRMS
.79068	.38593	.00000	.00000
1013 SPLIT_STRMS	1001 CSTR	1002 CSTR	1003 CSTR
.00000	.69642	.69534	.69471
1004 CSTR			
.00308			

Loop = 2	Run time (mins) = 24.48		
101 PASS_THRU	102 RELAX	111 ATTRITION	112 ATTRITION
.00000	.00322	.00000	.00000
113 ATTRITION	114 ATTRITION	120 MERGE_STRMS	201 LIFT_PIPE
.00000	.00000	.00322	.01806
301 ATTRITION	302 ATTRITION	303 ATTRITION	304 ATTRITION
.00000	.00000	.00000	.00000
321 ATTRITION	322 ATTRITION	323 ATTRITION	324 ATTRITION
.00000	.00000	.00000	.00000
330 MERGE_STRMS	310 MERGE_STRMS	401 CO_CURRENT	402 LIFT_PIPE
.02723	.00202	.01943	.00366
501 ATTRITION	502 ATTRITION	503 ATTRITION	512 MERGE_STRMS
.00000	.00000	.00000	.03484
513 MERGE_STRMS	514 MERGE_STRMS	521 ATTRITION	522 ATTRITION
.01656	.00414	.00000	.00000
523 ATTRITION	532 MERGE_STRMS	533 MERGE_STRMS	534 MERGE_STRMS
.00000	.03466	.01523	.01282
601 CSTR	611 SPLIT_STRMS	612 SPLIT_STRMS	613 SPLIT_STRMS
.00000	.00000	.00000	.00000

614	SPLIT_STRMS	621	CSTR	630	MERGE_STRMS	711	MERGE_STRMS
.00000		.00000		.01932		.00006	
712	MERGE_STRMS	713	MERGE_STRMS	714	MERGE_STRMS	801	MERGE_STRMS
.00005		.00004		.00002		.00018	
802	MERGE_STRMS	810	PHASE_CHANGE	811	MERGE_STRMS	812	SPLIT_STRMS
.01345		.00000		.00000		.00000	
820	SPLIT_STRMS	822	MERGE_STRMS	823	PHASE_CHANGE	821	SPLIT_STRMS
.00000		.00033		.00000		.00000	
824	PHASE_CHANGE	901	SPLIT_STRMS	913	FLUID_BED	912	FLUID_BED
.00000		.00000		.00293		.00333	
911	FLUID_BED	921	FLUID_BED	922	FLUID_BED	923	FLUID_BED
.00188		.00177		.00183		.00188	
930	MERGE_STRMS	940	CNTR_CURRENT	1011	SPLIT_STRMS	1012	SPLIT_STRMS
.00496		.00565		.00000		.00000	
1013	SPLIT_STRMS	1001	CSTR	1002	CSTR	1003	CSTR
.00000		.00213		.00218		.00219	
1004	CSTR						
	.00220						

N

Loop = 20	Run time (mins) = 164.97						
101	PASS_THRU	102	RELAX	111	ATTRITION	112	ATTRITION
.00000		.00001		.00000		.00000	
113	ATTRITION	114	ATTRITION	120	MERGE_STRMS	201	LIFT_PIPE
.00000		.00000		.00001		.00003	
301	ATTRITION	302	ATTRITION	303	ATTRITION	304	ATTRITION
.00000		.00000		.00000		.00000	
321	ATTRITION	322	ATTRITION	323	ATTRITION	324	ATTRITION
.00000		.00000		.00000		.00000	
330	MERGE_STRMS	310	MERGE_STRMS	401	CO_CURRENT	402	LIFT_PIPE
.00005		.00000		.00005		.00004	
501	ATTRITION	502	ATTRITION	503	ATTRITION	512	MERGE_STRMS
.00000		.00000		.00000		.00004	
513	MERGE_STRMS	514	MERGE_STRMS	521	ATTRITION	522	ATTRITION
.00001		.00003		.00000		.00000	
523	ATTRITION	532	MERGE_STRMS	533	MERGE_STRMS	534	MERGE_STRMS
.00000		.00011		.00005		.00005	
601	CSTR	611	SPLIT_STRMS	612	SPLIT_STRMS	613	SPLIT_STRMS
.00000		.00000		.00000		.00000	
614	SPLIT_STRMS	621	CSTR	630	MERGE_STRMS	711	MERGE_STRMS
.00000		.00000		.00006		.00002	
712	MERGE_STRMS	713	MERGE_STRMS	714	MERGE_STRMS	801	MERGE_STRMS
.00001		.00002		.00001		.00002	
802	MERGE_STRMS	810	PHASE_CHANGE	811	MERGE_STRMS	812	SPLIT_STRMS
.00001		.00000		.00000		.00000	
820	SPLIT_STRMS	822	MERGE_STRMS	823	PHASE_CHANGE	821	SPLIT_STRMS
.00000		.00001		.00000		.00000	
824	PHASE_CHANGE	901	SPLIT_STRMS	913	FLUID_BED	912	FLUID_BED
.00000		.00000		.00020		.00013	
911	FLUID_BED	921	FLUID_BED	922	FLUID_BED	923	FLUID_BED
.00008		.00005		.00003		.00002	
930	MERGE_STRMS	940	CNTR_CURRENT	1011	SPLIT_STRMS	1012	SPLIT_STRMS
.00000		.00004		.00000		.00000	
1013	SPLIT_STRMS	1001	CSTR	1002	CSTR	1003	CSTR
.00000		.00001		.00001		.00001	
1004	CSTR						
	.00001						

Loop = 21	Run time (mins) = 172.89						
101	PASS_THRU	102	RELAX	111	ATTRITION	112	ATTRITION
.00000		.00001		.00000		.00000	

113 ATTRITION	114 ATTRITION	120 MERGE_STRMS	201 LIFT_PIPE
.00000	.00000	.00001	.00002
301 ATTRITION	302 ATTRITION	303 ATTRITION	304 ATTRITION
.00000	.00000	.00000	.00000
321 ATTRITION	322 ATTRITION	323 ATTRITION	324 ATTRITION
.00000	.00000	.00000	.00000
330 MERGE_STRMS	310 MERGE_STRMS	401 CO_CURRENT	402 LIFT_PIPE
.00004	.00000	.00004	.00004
501 ATTRITION	502 ATTRITION	503 ATTRITION	512 MERGE_STRMS
.00000	.00000	.00000	.00004
513 MERGE_STRMS	514 MERGE_STRMS	521 ATTRITION	522 ATTRITION
.00001	.00002	.00000	.00000
523 ATTRITION	532 MERGE_STRMS	533 MERGE_STRMS	534 MERGE_STRMS
.00000	.00010	.00004	.00004
601 CSTR	611 SPLIT_STRMS	612 SPLIT_STRMS	613 SPLIT_STRMS
.00000	.00000	.00000	.00000
614 SPLIT_STRMS	621 CSTR	630 MERGE_STRMS	711 MERGE_STRMS
.00000	.00000	.00005	.00002
712 MERGE_STRMS	713 MERGE_STRMS	714 MERGE_STRMS	801 MERGE_STRMS
.00001	.00002	.00001	.00001
802 MERGE_STRMS	810 PHASE_CHANGE	811 MERGE_STRMS	812 SPLIT_STRMS
.00002	.00000	.00000	.00000
820 SPLIT_STRMS	822 MERGE_STRMS	823 PHASE_CHANGE	821 SPLIT_STRMS
.00000	.00001	.00000	.00000
824 PHASE_CHANGE	901 SPLIT_STRMS	913 FLUID_BED	912 FLUID_BED
.00000	.00000	.00018	.00012
911 FLUID_BED	921 FLUID_BED	922 FLUID_BED	923 FLUID_BED
.00007	.00004	.00003	.00002
930 MERGE_STRMS	940 CNTR_CURRENT	1011 SPLIT_STRMS	1012 SPLIT_STRMS
.00001	.00002	.00000	.00000
1013 SPLIT_STRMS	1001 CSTR	1002 CSTR	1003 CSTR
.00000	.00001	.00001	.00001
1004 CSTR			
.00001			

L

Module 8 : LIFT_PIPE Lift Pipe
Tag : 201 Group : 0 Version : 1.1

Gas stream	LFT_GIN	G201
-----	-----	-----
Stream number	1 in	10 out
Flow (mol/s)	6.03E-01	6.06E-01
Pressure (Pa)	1.57E+05	1.57E+05
Temperature (C)	499.85	565.49
Gas Composition (mol frac)		
N2	7.90E-01	7.86E-01
O2	2.10E-01	1.62E-01
H2	.00E+00	2.13E-04
CO2	.00E+00	4.10E-02
H2O	.00E+00	8.68E-03
H2S	.00E+00	1.18E-07
SO2	.00E+00	2.59E-04
NH3	.00E+00	3.27E-07
NO2	.00E+00	1.53E-03
CH4	.00E+00	5.07E-05
C2H4	.00E+00	3.55E-05
C3H6	.00E+00	2.20E-05
Oil-1	.00E+00	-3.36E-17
Oil-2	.00E+00	1.57E-17

Oil-3 .00E+00 -7.04E-18

Solid stream	S111A	S112B	S113C	S114D	M101A	M101B
Stream number	29 in	31 in	33 in	35 in	19 in	20 in
Flow (kg/min)	6.29E-01	4.27E-01	4.47E-01	3.66E-01	2.09E+00	2.56E+00
Temp (C)	503.63	503.62	503.63	503.65	503.67	503.66
Diameter (mm)	5.252	3.404	1.653	.389	4.772	3.175
Den (kg/m**3)	2023.2	2023.7	2025.9	2027.4	1946.8	1946.5
Porosity	.23842	.23811	.23677	.23586	.27754	.27935
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen-1	8.49E-05	1.58E-04	1.37E-04	1.12E-04	-4.51E-21	5.89E-24
Inert	4.72E-01	4.72E-01	4.71E-01	4.71E-01	4.92E-01	4.95E-01
CaCO3	2.48E-01	2.48E-01	2.48E-01	2.48E-01	2.57E-01	2.57E-01
CaO	-2.38E-42	3.62E-44	-1.91E-52	-2.89E-20	1.39E-05	1.54E-05
MgCO3	1.45E-01	1.45E-01	1.45E-01	1.45E-01	1.00E-01	9.33E-02
MgO	7.54E-05	7.01E-05	7.05E-05	7.11E-05	2.43E-02	2.81E-02
CaSiO3	1.27E-06	1.18E-06	1.20E-06	1.23E-06	2.18E-03	2.59E-03
SiO2	1.11E-01	1.11E-01	1.11E-01	1.11E-01	1.16E-01	1.18E-01
Oil-1	8.25E-05	7.64E-05	6.14E-05	5.79E-05	5.69E-05	5.85E-05
Oil-2	3.84E-04	4.34E-04	4.88E-04	4.64E-04	4.89E-04	4.83E-04
Oil-3	3.69E-04	5.11E-04	1.07E-03	1.25E-03	1.46E-03	1.39E-03
Coke	7.02E-04	7.00E-04	1.21E-03	1.82E-03	2.79E-03	2.71E-03
Char	2.18E-02	2.18E-02	2.18E-02	2.17E-02	3.60E-03	1.06E-03
Solid stream	M101C	M101D	F120	S201A	S201B	S201C
Stream number	21 in	22 in	37 in	38 out	39 out	40 out
Flow (kg/min)	1.05E+00	1.14E-01	3.39E-01	6.27E-01	4.24E-01	4.43E-01
Temp (C)	503.66	503.65	503.64	584.00	603.45	634.64
Diameter (mm)	1.667	.393	.050	5.252	3.404	1.653
Den (kg/m**3)	1954.7	1968.8	2025.9	2015.8	2013.8	2009.6
Porosity	.27484	.26867	.23678	.24290	.24408	.24659
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	9.03E-28	-2.82E-20	4.78E-04	6.97E-05	1.17E-04	7.30E-05
Kerogen-1	9.03E-28	-2.82E-20	4.78E-04	6.97E-05	1.17E-04	7.30E-05
Inert	4.89E-01	4.85E-01	4.71E-01	4.74E-01	4.74E-01	4.75E-01
CaCO3	2.56E-01	2.55E-01	2.48E-01	2.49E-01	2.49E-01	2.50E-01
CaO	4.75E-06	1.32E-06	-2.71E-21	6.66E-10	5.91E-10	5.08E-10
MgCO3	1.17E-01	1.33E-01	1.45E-01	1.46E-01	1.46E-01	1.46E-01
MgO	1.62E-02	7.79E-03	6.57E-05	8.07E-05	7.76E-05	8.41E-05
CaSiO3	1.37E-03	6.17E-04	1.10E-06	1.41E-06	1.41E-06	1.74E-06
SiO2	1.15E-01	1.14E-01	1.11E-01	1.11E-01	1.12E-01	1.12E-01
Oil-1	5.94E-05	5.95E-05	6.43E-05	7.71E-05	7.03E-05	5.49E-05
Oil-2	4.80E-04	4.77E-04	4.51E-04	3.59E-04	3.99E-04	4.36E-04
Oil-3	1.33E-03	1.29E-03	1.01E-03	3.44E-04	4.70E-04	9.54E-04
Coke	2.67E-03	2.56E-03	1.01E-03	2.44E-04	2.19E-04	3.12E-04
Char	6.13E-04	4.91E-05	2.17E-02	1.87E-02	1.76E-02	1.50E-02
Solid stream	S201D	M201A	M201B	M201C	M201D	F201
Stream number	41 out	42 out	43 out	44 out	45 out	46 out
Flow (kg/min)	3.63E-01	2.09E+00	2.56E+00	1.05E+00	1.14E-01	3.38E-01
Temp (C)	581.24	541.98	543.54	547.70	561.44	565.89
Diameter (mm)	.389	4.772	3.175	1.667	.393	.050
Den (kg/m**3)	2012.2	1944.1	1943.9	1952.1	1966.7	2016.9
Porosity	.24508	.27916	.28094	.27641	.26993	.24222
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00

O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	1.04E-04	-4.30E-21	5.63E-24	8.66E-28	-2.70E-20	4.63E-04
Kerogen-1	1.04E-04	-4.30E-21	5.63E-24	8.66E-28	-2.70E-20	4.63E-04
Inert	4.74E-01	4.92E-01	4.96E-01	4.90E-01	4.86E-01	4.73E-01
CaCO3	2.50E-01	2.57E-01	2.58E-01	2.56E-01	2.55E-01	2.49E-01
CaO	3.81E-10	1.39E-05	1.54E-05	4.76E-06	1.33E-06	2.43E-10
MgCO3	1.46E-01	1.01E-01	9.34E-02	1.17E-01	1.33E-01	1.46E-01
MgO	7.40E-05	2.43E-02	2.81E-02	1.62E-02	7.80E-03	6.70E-05
CaSiO3	1.30E-06	2.18E-03	2.59E-03	1.38E-03	6.18E-04	1.13E-06
SiO2	1.12E-01	1.17E-01	1.18E-01	1.15E-01	1.14E-01	1.11E-01
Oil-1	5.68E-05	5.60E-05	5.76E-05	5.86E-05	5.88E-05	6.36E-05
Oil-2	4.55E-04	4.81E-04	4.75E-04	4.73E-04	4.71E-04	4.46E-04
Oil-3	1.23E-03	1.44E-03	1.37E-03	1.31E-03	1.28E-03	9.95E-04
Coke	9.54E-04	1.59E-03	1.50E-03	1.49E-03	1.53E-03	7.10E-04
Char	1.53E-02	3.45E-03	9.45E-04	4.86E-04	3.67E-05	1.77E-02

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Overall balances for LIFT_PIPE , module 8
(in-out)/average in-out

Elemental C balance	8.12E-08	6.16E-10
Elemental H balance	-8.01E-09	-5.35E-13
Elemental O balance	9.90E-11	3.79E-12
Elemental N balance	9.23E-14	1.24E-15
Elemental S balance	-7.32E-14	-1.71E-18
Enthalpy balance	-1.08E-09	-8.61E-04

	in	out	
Solid Inorganic C	3.74E-01	3.74E-01	kg/min
Solid Inorganic C	.04662	.04674	wt. fraction
Solid Organic C	8.07E-02	6.27E-02	kg/min
Solid Organic C	.01005	.00783	wt. fraction

GAS-SOLID VELOCITIES ENTERING LIFT PIPE

NOTE: ENTRANCE CONDITIONS ARE USED
IN LIFT PIPE CALCULATIONS

GAS VELOCITY IN
9.73557

TOTAL SOLID VOLUME FRACTION IN
.00641

AVE SOLID VELOCITY IN
4.15495

INDEX	SLIP VELOCITY	SOLID VOL FRAC	SOLID VELOCITY	DIAMETER
1	6.21687	.00058	3.51869	.00525
2	5.77924	.00035	3.95632	.00340
3	5.12919	.00031	4.60637	.00165
4	3.62422	.00019	6.11134	.00039
5	6.08358	.00192	3.65198	.00477
6	5.67421	.00212	4.06136	.00317
7	5.11097	.00076	4.62460	.00167
8	3.61305	.00006	6.12252	.00039
9	.41940	.00012	9.31617	.00005

GAS-SOLID VELOCITIES BASED ON
EXIT CONDITIONS OF LIFT PIPE

GAS VELOCITY OUT

10.60781
 TOTAL SOLID VOLUME FRACTION OUT
 .00563
 AVE SOLID VELOCITY OUT
 4.73380
 INDEX SLIP VELOCITY SOLID VOL FRAC SOLID VELOCITY DIAMETER
 1 6.56727 .00050 4.04054 .00525
 2 6.09202 .00030 4.51578 .00340
 3 5.38528 .00028 5.22253 .00165
 4 3.73983 .00017 6.86797 .00039
 5 6.42540 .00168 4.18241 .00477
 6 5.98223 .00186 4.62558 .00317
 7 5.37097 .00067 5.23684 .00167
 8 3.73387 .00005 6.87393 .00039
 9 .39695 .00011 10.21086 .00005

N

 Module 55 : FLUID_BED Mixer Side 1 Top
 Tag : 913 Group : 0 Version : 1.0

Gas stream	G912	G913	B	55	1
Stream number	29	in	30	out	31 bub
Flow (mol/s)	4.77E-01		4.78E-01		2.88E-01
Pressure (Pa)	1.57E+05		1.57E+05		.00E+00
Temperature (C)	527.25		533.49		527.74
Gas Composition (mol frac)					
N2	8.06E-01		8.01E-01		8.03E-01
H2	9.02E-02		9.29E-02		9.19E-02
CO2	1.36E-03		1.52E-03		1.36E-03
H2O	2.58E-03		2.56E-03		2.55E-03
H2S	1.92E-03		1.90E-03		1.89E-03
NH3	1.05E-04		1.05E-04		1.03E-04
CH4	3.15E-02		3.23E-02		3.20E-02
C2H4	2.08E-02		2.12E-02		2.10E-02
C3H6	3.52E-02		3.55E-02		3.53E-02
Oil-1	8.17E-03		8.27E-03		8.21E-03
Oil-2	1.59E-03		1.51E-03		1.59E-03
Oil-3	1.08E-03		1.01E-03		1.08E-03

Solid stream	RAWA	RAWB	RAWC	RAWD	M711A	M712B
Stream number	1	in	2	in	3	in
Flow (kg/min)	7.60E-01		5.15E-01		5.39E-01	
Temp (C)	136.85		136.85		136.85	
Diameter (mm)	5.400		3.500		1.700	
Den (kg/m**3)	2247.0		2247.0		2247.0	
Porosity	.10000		.10000		.10000	
O Chr kg/m3	44.00		44.00		44.00	
O Ker kg/m3	272.00		272.00		272.00	
O FeS2 kg/m3	.00		.00		.00	
Solid Comp. (wt. frac.)						
Kerogen-1	1.21E-01		1.21E-01		1.21E-01	
Inert	4.25E-01		4.25E-01		4.25E-01	
CaCO3	2.23E-01		2.23E-01		2.23E-01	
CaO	.00E+00		.00E+00		.00E+00	
MgCO3	1.31E-01		1.31E-01		1.31E-01	
MgO	.00E+00		.00E+00		.00E+00	
CaSiO3	.00E+00		.00E+00		.00E+00	
SiO2	1.00E-01		1.00E-01		1.00E-01	

Oil-1	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Oil-2	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Oil-3	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Coke	.00E+00	.00E+00	.00E+00	.00E+00	2.34E-06	7.95E-07
Char	.00E+00	.00E+00	.00E+00	.00E+00	3.62E-03	1.07E-03
Solid stream	M713C	M714D	S913A	S913B	S913C	S913D
Stream number	131 in	132 in	133 out	134 out	135 out	136 out
Flow (kg/min)	1.04E+00	1.13E-01	7.60E-01	5.15E-01	5.39E-01	4.38E-01
Temp (C)	696.84	696.85	373.60	374.26	412.06	484.93
Diameter (mm)	1.667	.393	5.400	3.500	1.700	.400
Den (kg/m**3)	1945.1	1960.0	2246.9	2246.9	2246.4	2231.3
Porosity	.28038	.27386	.10008	.10005	.10037	.10988
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	.00E+00	.00E+00	1.21E-01	1.21E-01	1.20E-01	1.13E-01
Kerogen-1	.00E+00	.00E+00	1.21E-01	1.21E-01	1.20E-01	1.13E-01
Inert	4.91E-01	4.87E-01	4.25E-01	4.25E-01	4.25E-01	4.28E-01
CaCO3	2.57E-01	2.56E-01	2.24E-01	2.24E-01	2.24E-01	2.25E-01
CaO	4.18E-06	1.17E-06	.00E+00	.00E+00*****	.00E+00*****	.00E+00*****
MgCO3	1.18E-01	1.34E-01	1.31E-01	1.31E-01	1.31E-01	1.32E-01
MgO	1.61E-02	7.76E-03	6.27E-09	4.24E-09	2.20E-08	3.98E-07
CaSiO3	1.39E-03	6.21E-04	1.90E-11	1.30E-11	1.20E-10	5.42E-09
SiO2	1.16E-01	1.15E-01	1.00E-01	1.00E-01	1.00E-01	1.01E-01
Oil-1	.00E+00	.00E+00	1.22E-65	.00E+00*****	.00E+00*****	1.63E-41
Oil-2	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Oil-3	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Coke	4.79E-07	8.87E-07	1.12E-66	.00E+00*****	.00E+00*****	4.38E-42
Char	6.16E-04	4.93E-05	1.07E-05	7.25E-06	5.07E-05	1.36E-03
Solid stream	M913A	M913B	M913C	M913D		
Stream number	137 out	138 out	139 out	140 out		
Flow (kg/min)	2.09E+00	2.55E+00	1.05E+00	1.14E-01		
Temp (C)	599.19	599.37	588.61	561.90		
Diameter (mm)	4.772	3.176	1.667	.393		
Den (kg/m**3)	1936.6	1935.6	1946.9	1963.3		
Porosity	.28318	.28515	.27931	.27188		
O Chr kg/m3	44.00	44.00	44.00	44.00		
O Ker kg/m3	272.00	272.00	272.00	272.00		
O FeS2 kg/m3	.00	.00	.00	.00		
Solid Comp. (wt. frac.)						
Kerogen-1	-4.94E-20*****	-7.73E-91	1.46E-39			
Inert	4.94E-01	4.97E-01	4.91E-01	4.86E-01		
CaCO3	2.58E-01	2.59E-01	2.57E-01	2.55E-01		
CaO	1.19E-05	1.37E-05	4.17E-06	1.17E-06		
MgCO3	1.01E-01	9.39E-02	1.17E-01	1.34E-01		
MgO	2.43E-02	2.81E-02	1.61E-02	7.75E-03		
CaSiO3	2.21E-03	2.62E-03	1.39E-03	6.21E-04		
SiO2	1.17E-01	1.18E-01	1.16E-01	1.14E-01		
Oil-1	1.11E-04	1.17E-04	1.20E-04	1.10E-04		
Oil-2	1.11E-04	1.63E-04	2.81E-04	4.17E-04		
Oil-3	9.84E-05	1.62E-04	3.76E-04	1.04E-03		
Coke	1.89E-04	1.70E-04	1.74E-04	1.35E-04		
Char	3.62E-03	1.07E-03	6.16E-04	4.92E-05		

dp*scale = .21153D-02

AR = .33120D+07

Remf= 335.44370

Umf = .24243

Us/Umf = 9.71175

fb = .26095

Ub = 8.09351

Particle bed residence time information:

In Strm	Diam (mm)	In flow (kg/min)	Particle/volume	Vol Frac	Res. Time (s)
1	5.4000	7.596E-01	7.809E+05	.1171	13.56
2	3.5000	5.148E-01	1.269E+06	.0518	8.85
3	1.7000	5.388E-01	8.581E+06	.0401	6.55
4	.4000	4.410E-01	3.803E+08	.0232	4.62
5	4.7722	2.085E+00	3.605E+06	.3729	13.56
6	3.1762	2.553E+00	9.776E+06	.2982	8.85
7	1.6672	1.044E+00	2.037E+07	.0899	6.55
8	.3934	1.134E-01	1.179E+08	.0068	4.62

=====

Overall balances for FLUID_BED , module 55

(in-out)/average in-out

Elemental C balance	-8.87E-04	-1.07E-05
Elemental H balance	-4.02E-03	-3.61E-06
Elemental O balance	1.53E-05	5.15E-07
Elemental N balance	2.75E-03	3.00E-05
Elemental S balance	3.66E-03	3.33E-07
Enthalpy balance	-7.35E-06	-5.73E+00

	in	out	
Solid Inorganic C	3.66E-01	3.66E-01	kg/min
Solid Inorganic C	.04545	.04544	wt. fraction
Solid Organic C	2.37E-01	2.38E-01	kg/min
Solid Organic C	.02948	.02955	wt. fraction

N

Module 66 : CSTR Pyrolyzer Top
Tag : 1001 Group : 0 Version : 1.0

Gas stream	1G1011	G1001
Stream number	42	in
Flow (mol/s)	6.40E-03	1.87E-02
Pressure (Pa)	1.57E+05	1.57E+05
Temperature (C)	498.85	506.10
Gas Composition (mol frac)		
N2	7.96E-01	2.72E-01
H2	1.02E-01	1.60E-01
CO2	1.62E-03	1.94E-03
H2O	2.74E-03	4.83E-03
H2S	2.03E-03	3.51E-03
NH3	1.18E-04	2.34E-04
CH4	3.49E-02	5.40E-02
C2H4	2.30E-02	3.73E-02

C3H6	3.79E-02	6.07E-02
Oil-1	.00E+00	7.55E-02
Oil-2	.00E+00	2.30E-01
Oil-3	.00E+00	9.93E-02

Solid stream	S923A	S923B	S923C	S923D	M923A	M923B
Stream number	173 in	174 in	175 in	176 in	177 in	178 in
Flow (kg/min)	6.91E-01	4.73E-01	4.93E-01	4.03E-01	2.09E+00	2.56E+00
Temp (C)	519.63	519.49	522.62	523.84	524.97	524.97
Diameter (mm)	5.400	3.500	1.700	.400	4.772	3.176
Den (kg/m**3)	2043.4	2063.5	2057.7	2050.8	1941.1	1940.3
Porosity	.22621	.21401	.21754	.22169	.28052	.28233
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen-1	1.36E-02	2.51E-02	2.18E-02	1.79E-02	9.41E-19	-3.91E-30
Inert	4.67E-01	4.63E-01	4.64E-01	4.66E-01	4.93E-01	4.96E-01
CaCO3	2.46E-01	2.43E-01	2.44E-01	2.45E-01	2.57E-01	2.58E-01
CaO	-1.21E-96	-1.02E-96	-6.55E-93	-3.51E-92	1.19E-05	1.36E-05
MgCO3	1.44E-01	1.43E-01	1.43E-01	1.44E-01	1.01E-01	9.37E-02
MgO	1.55E-05	1.02E-05	1.07E-05	1.14E-05	2.43E-02	2.80E-02
CaSiO3	2.85E-07	1.89E-07	2.11E-07	2.41E-07	2.20E-03	2.62E-03
SiO2	1.10E-01	1.09E-01	1.09E-01	1.10E-01	1.16E-01	1.18E-01
Oil-1	5.19E-19	1.11E-17	-8.89E-20	1.61E-18	1.80E-04	1.54E-04
Oil-2	-2.12E-20	-3.89E-26	3.92E-19	1.46E-18	7.16E-04	7.54E-04
Oil-3	2.14E-52	.00E+00	-6.15E-57	.00E+00	9.65E-04	1.33E-03
Coke	4.74E-20	2.33E-19	8.03E-20	8.81E-19	9.70E-04	8.32E-04
Char	1.94E-02	1.73E-02	1.79E-02	1.86E-02	3.61E-03	1.06E-03
Solid stream	M923C	M923D	F940	S1001A	S1001B	S1001C
Stream number	179 in	180 in	181 in	182 out	183 out	184 out
Flow (kg/min)	1.05E+00	1.14E-01	1.96E-01	6.86E-01	4.67E-01	4.89E-01
Temp (C)	524.53	524.08	491.89	506.07	506.00	506.15
Diameter (mm)	1.667	.393	.050	5.400	3.500	1.700
Den (kg/m**3)	1951.7	1966.6	2241.1	2030.7	2039.9	2037.2
Porosity	.27644	.26994	.10373	.23388	.22831	.22995
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	-2.33E-27	1.11E-22	1.18E-01	6.27E-03	1.16E-02	1.01E-02
Kerogen-1	-2.33E-27	1.11E-22	1.18E-01	6.27E-03	1.16E-02	1.01E-02
Inert	4.90E-01	4.86E-01	4.26E-01	4.70E-01	4.68E-01	4.69E-01
CaCO3	2.56E-01	2.55E-01	2.24E-01	2.47E-01	2.46E-01	2.47E-01
CaO	4.16E-06	1.16E-06	-1.51E-71	5.38E-86	4.54E-86	2.36E-82
MgCO3	1.17E-01	1.33E-01	1.31E-01	1.45E-01	1.44E-01	1.44E-01
MgO	1.61E-02	7.75E-03	1.37E-07	2.18E-05	1.66E-05	1.71E-05
CaSiO3	1.38E-03	6.20E-04	2.03E-09	3.94E-07	2.98E-07	3.20E-07
SiO2	1.15E-01	1.14E-01	1.00E-01	1.11E-01	1.10E-01	1.10E-01
Oil-1	1.27E-04	1.18E-04	.00E+00	2.62E-08	9.33E-18	1.06E-10
Oil-2	6.89E-04	6.55E-04	.00E+00	1.15E-07	-2.50E-19	4.65E-10
Oil-3	1.82E-03	1.97E-03	.00E+00	5.66E-08	-1.86E-24	2.29E-10
Coke	7.92E-04	6.14E-04	.00E+00	2.63E-08	1.33E-18	1.06E-10
Char	6.14E-04	4.91E-05	5.12E-04	2.07E-02	1.97E-02	2.00E-02
Solid stream	S1001D	M1001A	M1001B	M1001C	M1001D	F1001
Stream number	185 out	186 out	187 out	188 out	189 out	190 out
Flow (kg/min)	3.99E-01	2.10E+00	2.57E+00	1.05E+00	1.14E-01	1.85E-01
Temp (C)	506.12	506.18	506.16	506.15	506.11	506.06
Diameter (mm)	.400	4.772	3.176	1.667	.393	.050

Den (kg/m**3)	2034.1	1948.3	1946.9	1957.5	1972.2	2121.1
Porosity	.23184	.27623	.27840	.27295	.26656	.17864
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	8.24E-03	4.28E-19	-7.87E-30	-8.60E-27	2.13E-22	5.69E-02
Kerogen-1	8.24E-03	4.28E-19	-7.87E-30	-8.60E-27	2.13E-22	5.69E-02
Inert	4.69E-01	4.91E-01	4.94E-01	4.88E-01	4.84E-01	4.50E-01
CaCO3	2.47E-01	2.56E-01	2.57E-01	2.56E-01	2.54E-01	2.37E-01
CaO	1.39E-71	1.18E-05	1.36E-05	4.15E-06	1.16E-06	-1.58E-71
MgCO3	1.45E-01	1.00E-01	9.33E-02	1.17E-01	1.33E-01	1.39E-01
MgO	1.78E-05	2.42E-02	2.79E-02	1.61E-02	7.74E-03	6.13E-06
CaSiO3	3.51E-07	2.19E-03	2.61E-03	1.38E-03	6.18E-04	1.05E-07
SiO2	1.10E-01	1.16E-01	1.17E-01	1.15E-01	1.14E-01	1.06E-01
Oil-1	6.46E-08	2.02E-05	1.97E-05	1.93E-05	1.91E-05	.00E+00
Oil-2	2.88E-07	1.71E-03	1.69E-03	1.67E-03	1.65E-03	.00E+00
Oil-3	1.42E-07	3.36E-03	3.43E-03	3.45E-03	3.43E-03	.00E+00
Coke	6.58E-08	1.42E-03	1.31E-03	1.27E-03	1.11E-03	.00E+00
Char	2.03E-02	3.60E-03	1.06E-03	6.12E-04	4.90E-05	1.15E-02

Liquid stream	L812	LDUM
Stream number	5	in
Flow (kg/min)	1.50E-01	5.72E-04
Temperature	141.85	506.10
Liq Composition (wt frac)		
Oil-2	5.99E-01	5.99E-01
Oil-3	4.01E-01	4.01E-01

Particle bed residence time information:

In Strm	Diam (mm)	In flow (kg/min)	Particle/volume	Vol Frac	Res. Time (s)
1	5.4000	6.908E-01	5.525E+05	.0828	21.59
2	3.5000	4.728E-01	1.375E+06	.0561	21.59
3	1.7000	4.934E-01	1.256E+07	.0587	21.59
4	.4000	4.025E-01	7.892E+08	.0481	21.59
5	4.7722	2.091E+00	2.550E+06	.2639	21.59
6	3.1762	2.560E+00	1.060E+07	.3233	21.59
7	1.6672	1.048E+00	2.982E+07	.1315	21.59
8	.3934	1.138E-01	2.446E+08	.0142	21.59
9	.0500	1.957E-01	1.798E+11	.0214	21.59

=====

Overall balances for CSTR , module 66

	(in-out)/average	in-out
Elemental C balance	-3.29E-06	-3.36E-08
Elemental H balance	3.90E-05	1.72E-08
Elemental O balance	1.17E-07	4.01E-09
Elemental N balance	3.46E-05	9.30E-09
Elemental S balance	1.22E-04	5.77E-09
Enthalpy balance	-4.91E-09	-3.97E-03

	in	out
Solid Inorganic C	3.75E-01	3.75E-01
Solid Inorganic C	.04644	.04648
Solid Organic C	1.11E-01	1.04E-01
Solid Organic C	.01370	.01290
		kg/min
		wt. fraction
		kg/min
		wt. fraction

APPENDIX C

EXAMPLE: A SUMMARY

For very large simulation runs it is often convenient to have an input file setup to extract certain summary information about the run without including all the detailed information. The ASCII file generated during the run includes output from every module and can be quite long. In addition, certain summary information is not required by the basic simulation and computing it during the actual run just increases the number of modules and the size of the output files. In this example a summary run is outlined which was designed to extract certain information from the results of the lengthy example described in Appendix B. The ".strm" file from the full simulation must be retained for input to this summary run. In the dialogue between OSP and the user that initiates a run the question "Initialize streams from file ? (def = n)" must be answered "yes" and then the last entry in the base run's stream file selected.

A listing of the complete input file is given in the "**INPUT FILE**" section below. The file consists only of a \$GLOBAL and several \$MODULE sections.. In the \$GLOBAL input the LOOPMAX parameter is set to one since no iteration is required and the CHECK_CON variable is set to zero so that stream connectivity checks are not performed. They would be meaningless for this application.

The remainder of the input file consists of MERGE_STRMS and BALANCE modules which are used to give information on various overall aspects of the simulation. The intent of each module is described by its title.

A listing of selected portions of the ASCII output file for this example are given in the final section of this Appendix. In the title portion of the output information is given about the input stream file used in the run. This was the stream file generated by the problem described in Appendix B.

Following the title section the next portion of the file shown is the results section of the first module, a MERGE_STRMS module used to collect together the combined combustion gas streams. Next, another MERGE_STRMS result is shown in which the composite flow, composition and temperature of solids sent to the spent hopper is computed. The next listed module is again a MERGE_STRMS module showing the combined raw shale input rate. This is followed by a BALANCE module which presents information on the overall pyrolysis process in the FBM & PYR. The final results shown are for another BALANCE module. This one is used to determine the extent of heating/cooling of all recycle particle streams. Since the gas stream doing the heating/cooling has not been included in the input/output streams, the balance section can be used to determine the net heating/cooling, -2.26 kW. Since the value is negative and the difference is defined of input streams minus output streams there is a net heating of recycle material.

INPUT FILE

```

*
*
$GLOBAL    loopmax=1
            title='Summary Information for Run (Includes Oil/gas Recycle)'
            check_con=0

*****
*   Module definition section.  Keywords required (no spaces in keywords).
*****

*****
$MODULE = MERGE_STRMS desc= 'Combined Combustion Gas'
go(1)=CMB_GOUT gi(1)=FBC_GOUT gi(1)=DFC_GOUT
*****


*** Just display these streams
$MODULE = MERGE_STRMS desc= 'Gases: LFT,DFC,DFC-A,FBC-T,FBC-B,FBM-BOut'
go=GDUM1
gi=G201 gi=G401 gi=DFC_GOUT gi=FBC_GOUT gi=G621 gi=G930

*****


$MODULE = MERGE_STRMS desc= 'Total Solids to Spent Hopper'
so(1)=SPENT
si(1)=SA_SOUT si(1)=SB_SOUT si(1)=SC_SOUT si(1)=SD_SOUT
si(1)=MA_SOUT si(1)=MB_SOUT si(1)=MC_SOUT si(1)=MD_SOUT
si(1)=DFC_FOUT
*****


$MODULE = MERGE_STRMS desc= 'Total Raw Feed'
so(1)=RAW
si(1)=RAWA si(1)=RAWB si(1)=RAWC si(1)=RAWD
si(1)=FRAW
*****


$MODULE = MERGE_STRMS desc= 'Total Pyrolyzer Out Solids'
so(1)=PYR
si(1)=S1004A si(1)=S1004B si(1)=S1004C si(1)=S1004D
si(1)=M1004A si(1)=M1004B si(1)=M1004C si(1)=M1004D
si(1)=F1004
*****


$MODULE = MERGE_STRMS desc= 'Total LFT Out Solids'
so(1)=LFT
si(1)=S201A si(1)=S201B si(1)=S201C si(1)=S201D
si(1)=M201A si(1)=M201B si(1)=M201C si(1)=M201D
si(1)=F201
*****


$MODULE = MERGE_STRMS desc= 'Total DFC Out Solids'
so(1)=DFC
si(1)=S401A si(1)=S401B si(1)=S401C si(1)=S401D
si(1)=M401A si(1)=M401B si(1)=M401C si(1)=M401D
si(1)=F401
*****


$MODULE = MERGE_STRMS desc= 'Total FBC Solids Out'
so(1)=FBC
si(1)=S621A si(1)=S621B si(1)=S621C si(1)=S621D
si(1)=M621A si(1)=M621B si(1)=M621C si(1)=M621D
*****


$MODULE = BALANCE      desc= 'Overall Oil/Coking in FBM & PYR'
gi=GN2MAKE

```

```

go=PYR_GOUT
lo=1_LOUT lo=2&3_LOUT
si=RAWA    si=RAWB    si=RAWC    si=RAWD
si=M711A   si=M712B   si=M713C   si=M714D
si=FRAW
so=S1004A  so=S1004B  so=S1004C  so=S1004D
so=M1004A  so=M1004B  so=M1004C  so=M1004D
so=F1004
*****
$MODULE = BALANCE      desc= 'Overall Oil/Coking in FBM '
gi=G723
go=G840
si=RAWA    si=RAWB    si=RAWC    si=RAWD
si=M711A   si=M712B   si=M713C   si=M714D
si=FRAW
so=S923A   so=S923B   so=S923C   so=S923D
so=M923A   so=M923B   so=M923C   so=M923D
so=F940
*****
$MODULE = BALANCE      desc= 'Overall Oil/Coking in PYR'
gi=G724
go=G701
li=L712
si=S923A   si=S923B   si=S923C   si=S923D
si=M923A   si=M923B   si=M923C   si=M923D
si=F940
so=S1004A  so=S1004B  so=S1004C  so=S1004D
so=M1004A  so=M1004B  so=M1004C  so=M1004D
so=F1004
*****
$MODULE = BALANCE      desc= 'Heating/Cooling & Recycle Particle Dist.'
si=S621A   si=S621B   si=S621C   si=S621D
si=M621A   si=M621B   si=M621C   si=M621D
so=M711A   so=M712B   so=M713C   so=M714D
*****
$MODULE = BALANCE      desc= 'Recycle Particle Distribution'
si=M711A   si=M712B   si=M713C   si=M714D
*****
$MODULE = BALANCE      desc= 'PYR Particle Distribution'
si=S111A   si=S112B   si=S113C   si=S114D
si=M101A   si=M101B   si=M101C   si=M101D
si=F120
*****
$MODULE = BALANCE      desc= 'Spent Particle Distribution'
si=SA_SOUT  si=SB_SOUT  si=SC_SOUT  si=SD_SOUT
si=MA_SOUT  si=MB_SOUT  si=MC_SOUT  si=MD_SOUT
si=DFC_FOUT
so= SDUM1

```

OUTPUT FILE

Selected portions of the ASCII output file for the example run are given below.

%%%%%%%%%%%%%%
%%%%%%%%%%%%%

Title : Summary Information for Run (Includes Oil/gas Recycle)

Input file: sum.inp

Input from stream file: h20.strm
[After loop 22 Module No. 69
Module: CSTR
Title: Lab Retort H20 - 9P Sizes
Date: 30-Nov-93
Time: 09:02:03]

Time : 14:14:44
Date : 30-Nov-93

Model : osp
Version: 2.0
Machine: HP-9000

%%%%%%%%%%%%%%
%%%%%%%%%%%%%

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Module 1 : MERGE_STRMS Combined Combustion Gas
Tag : Group : 0 Version : 1.0

Gas stream	CMB_GOUT	FBC_GOUT	DFC_GOUT
-----	-----	-----	-----
Stream number	48 out	14 in	12 in
Flow (mol/s)	1.07E+00	4.52E-01	6.14E-01
Pressure (Pa)	1.57E+05	1.57E+05	1.57E+05
Temperature (C)	678.27	661.21	690.28
Gas Composition (mol frac)			
N2	8.31E-01	9.05E-01	7.76E-01
O2	6.09E-02	2.66E-02	8.62E-02
H2	2.02E-03	.00E+00	3.50E-03
CO2	8.56E-02	5.81E-02	1.06E-01
H2O	1.64E-02	8.23E-03	2.25E-02
H2S	1.12E-06	.00E+00	1.94E-06
SO2	5.16E-04	2.88E-04	6.83E-04
NH3	3.10E-06	.00E+00	5.38E-06
NO2	2.96E-03	1.57E-03	3.98E-03
CH4	4.80E-04	.00E+00	8.33E-04
C2H4	3.36E-04	.00E+00	5.83E-04
C3H6	2.08E-04	.00E+00	3.61E-04
Oil-2	8.94E-18	.00E+00	1.55E-17

=====

Overall balances for MERGE_STRMS , module 1

	(in-out)/average	in-out	
Elemental C balance	.00E+00	.00E+00	
Elemental H balance	1.53E-16	6.78E-21	
Elemental O balance	.00E+00	.00E+00	
Elemental N balance	1.40E-16	3.47E-18	
Elemental S balance	.00E+00	.00E+00	
Enthalpy balance	-3.63E-11	-6.45E-07	
	in	out	
Solid Inorganic C	.00E+00	.00E+00	kg/min
Solid Inorganic C	.00000	.00000	wt. fraction
Solid Organic C	.00E+00	.00E+00	kg/min
Solid Organic C	.00000	.00000	wt. fraction

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Module 3 : MERGE_STRMS Total Solids to Spent Hopper
Tag : Group : 0 Version : 1.0

Solid stream	SPENT	SA_SOUT	SB_SOUT	SC_SOUT	SD_SOUT	MA_SOUT
Stream number	209 out	106 in	110 in	114 in	118 in	108 in
Flow (kg/min)	2.13E+00	3.22E-02	2.36E-02	1.68E-01	4.11E-01	1.81E-01
Temp (C)	670.47	678.96	679.55	674.77	664.90	652.54
Diameter (mm)	1.311	4.955	3.302	1.664	.392	4.740
Den (kg/m**3)	1958.5	1996.5	1990.8	1985.2	1977.9	1935.1
Porosity	.27385	.25239	.25580	.26015	.26539	.28430
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen-1	4.35E-07	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Inert	4.88E-01	4.77E-01	4.78E-01	4.80E-01	4.83E-01	4.95E-01
CaCO3	2.56E-01	2.51E-01	2.51E-01	2.53E-01	2.54E-01	2.58E-01
CaO	4.46E-06	6.70E-10	6.15E-10	5.59E-10	4.26E-10	1.39E-05
MgCO3	1.29E-01	1.43E-01	1.43E-01	1.45E-01	1.48E-01	9.99E-02
MgO	1.02E-02	1.93E-03	2.16E-03	1.58E-03	5.25E-04	2.50E-02
CaSiO3	8.94E-04	1.25E-04	1.45E-04	1.00E-04	2.75E-05	2.24E-03
SiO2	1.15E-01	1.12E-01	1.12E-01	1.13E-01	1.14E-01	1.17E-01
Oil-1	6.67E-06	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Oil-2	4.40E-05	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Oil-3	9.17E-05	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00
Coke	6.73E-05	3.94E-06	1.99E-06	3.18E-06	3.14E-05	1.20E-04
Char	1.88E-03	1.56E-02	1.28E-02	7.71E-03	1.72E-03	3.00E-03
Solid stream	MB_SOUT	MC_SOUT	MD_SOUT	DFC_FOUT		
Stream number	112 in	116 in	120 in	74 in		
Flow (kg/min)	1.73E-01	3.69E-01	1.79E-01	5.98E-01		
Temp (C)	657.26	659.83	659.79	690.34		
Diameter (mm)	3.159	1.669	.396	.050		
Den (kg/m**3)	1935.0	1942.2	1951.7	1960.4		
Porosity	.28593	.28196	.27769	.27259		
O Chr kg/m3	44.00	44.00	44.00	44.00		
O Ker kg/m3	272.00	272.00	272.00	272.00		
O FeS2 kg/m3	.00	.00	.00	.00		
Solid Comp. (wt. frac.)						
Kerogen tot	.00E+00	.00E+00	.00E+00	1.55E-06		
Kerogen-1	.00E+00	.00E+00	.00E+00	1.55E-06		
Inert	4.98E-01	4.93E-01	4.90E-01	4.85E-01		

CaCO3	2.59E-01	2.58E-01	2.57E-01	2.55E-01
CaO	1.55E-05	6.05E-06	3.83E-06	2.34E-06
MgCO3	9.27E-02	1.14E-01	1.24E-01	1.40E-01
MgO	2.88E-02	1.82E-02	1.30E-02	4.48E-03
CaSiO3	2.65E-03	1.56E-03	1.09E-03	3.98E-04
SiO2	1.19E-01	1.16E-01	1.15E-01	1.14E-01
Oil-1	.00E+00	.00E+00	.00E+00	2.38E-05
Oil-2	.00E+00	.00E+00	.00E+00	1.57E-04
Oil-3	.00E+00	.00E+00	.00E+00	3.27E-04
Coke	3.96E-05	2.97E-05	6.37E-05	1.33E-04
Char	5.46E-04	1.28E-04	6.22E-05	8.45E-04

=====

Overall balances for MERGE_STRMS , module 3
 (in-out)/average in-out

Elemental C balance	2.40E-16	4.34E-19
Elemental H balance	.00E+00	.00E+00
Elemental O balance	1.86E-16	1.73E-18
Elemental N balance	-1.38E-16	-4.24E-22
Elemental S balance	.00E+00	.00E+00
Enthalpy balance	-1.32E-10	-2.77E-05

	in	out	
Solid Inorganic C	1.05E-01	1.05E-01	kg/min
Solid Inorganic C	.04899	.04899	wt. fraction
Solid Organic C	3.93E-03	3.93E-03	kg/min
Solid Organic C	.00184	.00184	wt. fraction

Module 4 : MERGE_STRMS Total Raw Feed
 Tag : Group : 0 Version : 1.0

Solid stream	RAW	RAWA	RAWB	RAWC	RAWD	FRAW
Stream number	210 out	1 in	2 in	3 in	4 in	5 in
Flow (kg/min)	2.45E+00	7.60E-01	5.15E-01	5.39E-01	4.41E-01	1.96E-01
Temp (C)	136.85	136.85	136.85	136.85	136.85	136.85
Diameter (mm)	2.859	5.400	3.500	1.700	.400	.050
Den (kg/m***3)	2247.0	2247.0	2247.0	2247.0	2247.0	2247.0
Porosity	.10000	.10000	.10000	.10000	.10000	.10000
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen tot	1.21E-01	1.21E-01	1.21E-01	1.21E-01	1.21E-01	1.21E-01
Kerogen-1	1.21E-01	1.21E-01	1.21E-01	1.21E-01	1.21E-01	1.21E-01
Inert	4.25E-01	4.25E-01	4.25E-01	4.25E-01	4.25E-01	4.25E-01
CaCO3	2.23E-01	2.23E-01	2.23E-01	2.23E-01	2.23E-01	2.23E-01
MgCO3	1.31E-01	1.31E-01	1.31E-01	1.31E-01	1.31E-01	1.31E-01
SiO2	1.00E-01	1.00E-01	1.00E-01	1.00E-01	1.00E-01	1.00E-01

=====

Overall balances for MERGE_STRMS , module 4
 (in-out)/average in-out

Elemental C balance	.00E+00	.00E+00
Elemental H balance	-2.10E-16	-1.08E-19
Elemental O balance	.00E+00	.00E+00
Elemental N balance	1.13E-16	1.36E-20
Elemental S balance	.00E+00	.00E+00
Enthalpy balance	.00E+00	.00E+00

	in	out	
Solid Inorganic C	1.11E-01	1.11E-01	kg/min
Solid Inorganic C	.04547	.04547	wt. fraction
Solid Organic C	2.47E-01	2.47E-01	kg/min
Solid Organic C	.10099	.10099	wt. fraction

Module 5 : MERGE_STRMS Total Pyrolyzer Out Solids
Tag : Group : 0 Version : 1.0

Solid stream	PYR	S1004A	S1004B	S1004C	S1004D	M1004A
Stream number	211 out	6 in	7 in	8 in	9 in	11 in
Flow (kg/min)	8.03E+00	6.84E-01	4.64E-01	4.86E-01	3.98E-01	2.09E+00
Temp (C)	503.66	503.63	503.63	503.64	503.66	503.68
Diameter (mm)	3.268	5.400	3.500	1.700	.400	4.772
Den (kg/m**3)	1967.9	2023.2	2023.7	2025.9	2027.4	1944.8
Porosity	.26720	.23842	.23811	.23677	.23585	.27827
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Kerogen-1	4.82E-05	8.55E-05	1.60E-04	1.37E-04	1.12E-04	5.76E-21
Inert	4.87E-01	4.72E-01	4.72E-01	4.71E-01	4.71E-01	4.92E-01
CaCO3	2.54E-01	2.48E-01	2.48E-01	2.48E-01	2.48E-01	2.57E-01
CaO	8.03E-06	-3.92E-44	3.86E-47	-2.03E-55	-7.49E-19	1.19E-05
MgCO3	1.13E-01	1.45E-01	1.45E-01	1.45E-01	1.45E-01	1.01E-01
MgO	1.75E-02	7.53E-05	7.01E-05	7.05E-05	7.11E-05	2.43E-02
CaSiO3	1.60E-03	1.27E-06	1.18E-06	1.20E-06	1.23E-06	2.20E-03
SiO2	1.15E-01	1.11E-01	1.11E-01	1.11E-01	1.11E-01	1.16E-01
Oil-1	6.16E-05	8.26E-05	7.66E-05	6.15E-05	5.79E-05	5.71E-05
Oil-2	4.72E-04	3.83E-04	4.34E-04	4.89E-04	4.64E-04	4.90E-04
Oil-3	1.24E-03	3.68E-04	5.10E-04	1.07E-03	1.25E-03	1.47E-03
Coke	2.26E-03	6.98E-04	6.98E-04	1.21E-03	1.82E-03	2.79E-03
Char	7.34E-03	2.18E-02	2.18E-02	2.18E-02	2.17E-02	3.61E-03
Solid stream	M1004B	M1004C	M1004D	F1004		
Stream number	12 in	13 in	14 in	10 in		
Flow (kg/min)	2.56E+00	1.05E+00	1.14E-01	1.77E-01		
Temp (C)	503.67	503.67	503.66	503.66		
Diameter (mm)	3.176	1.667	.393	.050		
Den (kg/m**3)	1943.4	1953.8	1968.5	2026.9		
Porosity	.28053	.27518	.26877	.23616		
O Chr kg/m3	44.00	44.00	44.00	44.00		
O Ker kg/m3	272.00	272.00	272.00	272.00		
O FeS2 kg/m3	.00	.00	.00	.00		
Solid Comp. (wt. frac.)						
Kerogen tot	4.70E-31	-2.30E-22	-8.49E-24	8.08E-04		
Kerogen-1	4.70E-31	-2.30E-22	-8.49E-24	8.08E-04		
Inert	4.95E-01	4.89E-01	4.85E-01	4.71E-01		
CaCO3	2.57E-01	2.56E-01	2.55E-01	2.48E-01		
CaO	1.37E-05	4.18E-06	1.17E-06	-2.81E-62		
MgCO3	9.34E-02	1.17E-01	1.33E-01	1.45E-01		
MgO	2.80E-02	1.62E-02	7.80E-03	5.98E-05		
CaSiO3	2.62E-03	1.38E-03	6.20E-04	9.86E-07		
SiO2	1.18E-01	1.15E-01	1.14E-01	1.11E-01		
Oil-1	5.86E-05	5.95E-05	5.96E-05	5.80E-05		
Oil-2	4.84E-04	4.81E-04	4.78E-04	4.64E-04		
Oil-3	1.40E-03	1.33E-03	1.29E-03	1.25E-03		
Coke	2.71E-03	2.67E-03	2.56E-03	9.84E-04		
Char	1.06E-03	6.14E-04	4.91E-05	2.16E-02		

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Overall balances for MERGE_STRMS , module 5
(in-out)/average in-out

Elemental C balance	1.14E-16	8.67E-19
Elemental H balance	.00E+00	.00E+00
Elemental O balance	4.05E-16	1.39E-17
Elemental N balance	-2.33E-16	-1.36E-20
Elemental S balance	.00E+00	.00E+00
Enthalpy balance	-1.40E-11	-1.13E-05

	in	out	
Solid Inorganic C	3.75E-01	3.75E-01	kg/min
Solid Inorganic C	.04664	.04664	wt. fraction
Solid Organic C	8.07E-02	8.07E-02	kg/min
Solid Organic C	.01005	.01005	wt. fraction

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Module 8 : MERGE_STRMS Total FBC Solids Out
Tag : Group : 0 Version : 1.0

Solid stream	FBC	S621A	S621B	S621C	S621D	M621A
Stream number	214 out	121 in	122 in	123 in	124 in	125 in
Flow (kg/min)	5.80E+00	3.13E-01	3.05E-01	3.25E-01	7.89E-02	1.77E+00
Temp (C)	680.25	692.77	691.71	686.81	679.53	678.36
Diameter (mm)	3.424	4.955	3.302	1.664	.392	4.740
Den (kg/m**3)	1937.4	1978.6	1971.1	1964.7	1966.6	1928.2
Porosity	.28383	.26150	.26604	.27099	.27087	.28761
O Chr kg/m3	44.00	44.00	44.00	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00	.00	.00	.00
Solid Comp. (wt. frac.)						
Inert	4.95E-01	4.81E-01	4.83E-01	4.85E-01	4.85E-01	4.96E-01
CaCO3	2.58E-01	2.53E-01	2.54E-01	2.55E-01	2.55E-01	2.59E-01
CaO	1.11E-05	6.76E-10	6.21E-10	5.65E-10	4.28E-10	1.40E-05
MgCO3	1.02E-01	1.35E-01	1.35E-01	1.38E-01	1.41E-01	9.54E-02
MgO	2.42E-02	6.58E-03	6.70E-03	5.70E-03	4.14E-03	2.74E-02
CaSiO3	2.21E-03	5.22E-04	5.30E-04	4.32E-04	2.97E-04	2.50E-03
SiO2	1.17E-01	1.13E-01	1.13E-01	1.14E-01	1.14E-01	1.17E-01
Coke	1.29E-06	7.52E-08	3.85E-08	6.49E-08	6.74E-07	2.74E-06
Char	1.89E-03	1.19E-02	8.03E-03	1.96E-03	6.98E-05	2.17E-03

Solid stream	M621B	M621C	M621D
Stream number	126 in	127 in	128 in
Flow (kg/min)	2.25E+00	7.19E-01	3.45E-02
Temp (C)	677.90	678.15	678.95
Diameter (mm)	3.159	1.669	.396
Den (kg/m**3)	1929.5	1936.2	1944.9
Porosity	.28848	.28464	.28069
O Chr kg/m3	44.00	44.00	44.00
O Ker kg/m3	272.00	272.00	272.00
O FeS2 kg/m3	.00	.00	.00
Solid Comp. (wt. frac.)			
Inert	4.99E-01	4.94E-01	4.92E-01
CaCO3	2.59E-01	2.58E-01	2.57E-01
CaO	1.55E-05	6.07E-06	3.84E-06
MgCO3	8.85E-02	1.09E-01	1.18E-01

MgO	3.10E-02	2.09E-02	1.60E-02
CaSiO ₃	2.91E-03	1.82E-03	1.36E-03
SiO ₂	1.19E-01	1.16E-01	1.16E-01
Coke	8.98E-07	6.67E-07	1.37E-06
Char	1.24E-04	6.39E-06	2.40E-06

=====

Overall balances for MERGE_STRMS , module 8	
	(in-out)/average in-out
Elemental C balance	.00E+00 .00E+00
Elemental H balance	.00E+00 .00E+00
Elemental O balance	.00E+00 .00E+00
Elemental N balance	.00E+00 .00E+00
Elemental S balance	1.22E-16 4.24E-22
Enthalpy balance	-4.03E-11 -2.27E-05
	in out
Solid Inorganic C	2.63E-01 2.63E-01
Solid Inorganic C	.04544 .04544
Solid Organic C	9.66E-03 9.66E-03
Solid Organic C	.00167 .00167
	kg/min wt. fraction

N

APPENDIX D

EXAMPLE: USING STOICH MODULE

This is an example which uses STOICH modules. The module is used to help determine the stoichiometric coefficients for two different reaction. The input file is listed in the "INPUT FILE" section and selected portions of the output file are listed in the "OUTPUT FILE" section.

In the \$GLOBAL section of the input file, LOOPMAX is set to one, since no iteration is required, and CHECK_CON is set to zero so that no stream connectivity check is done.

The first STOICH module is setup to determine the stoichiometric coefficients of coke combustion and to compute its heat of reaction between 273 & 1273 °K. The stoichiometry is to be based on the solid component COKE having a coefficient of one. All five possible atomic balances are to be used to determine the stoichiometric coefficients for four gaseous combustion products and oxygen. Notice that the solid weight fraction of COKE has been set to negative one. This is done because the STOICH module uses the stream variables in a special way. Negative numbers are used to indicate reactants.

The next module is setup to balance an overall pyrolysis reaction for KEROGEN-1. Again all five atomic balances are used. The five unknowns to be determined are stoichiometric coefficients for two gas products (H₂ & C₂H₆) and three solid species (CHAR-S, CHAR-N, and CHAR-O). In this case eight gas species coefficients are set through the use of the GAS2 stream initialization.

Notice that in this example the \$MODULE and \$INIT- sections have been intermixed. This was done to allow a more logical grouping. Remember that the order of the different input sections is only important in that the order of \$MODULE definitions will determine the order of their computation.

In the ASCII output file listing given below the portions of the \$PROPERTY section are listed which give the composition information for the gas and solid species. Following this portion of the output file, the computed results from the first STOICH module are listed. Although perhaps not clear in this listing, the results of the STOICH module calculations appear in a slightly different place in the output file than for most other modules. Because the module was not intended to simulate some physical operation, but rather to compute stoichiometric coefficients, it operates differently than most other modules. All calculations are done during the initialization portion of the OSP simulation. The computed results are available and are output to the ASCII output file at the time the other modules are simply listing their input parameters. As a result, the listing includes both input information as well as computed results. Note, also as a consequence of the way this module operates, it does not recompute coefficients as a result of changes in stream variables made by other modules.

The computed stoichiometric coefficients are given in terms of "Internal Units" and mass based units. The term "Internal Units" refers to the units used by OSP for input of compositional information. This is mass based for solids and liquids and mole based for gases.

Consequently, for solid and liquid species, the values in the two columns will be the same but for gases they will differ since in the first column coefficients will be given in mole (gram mole) units. The negative numbers indicate reactant species.

Results for the second module, which computes the stoichiometric coefficients for kerogen pyrolysis, completes the output listing.

INPUT FILE

Listing of full input file for this example is given below.

```
$GLOBAL      title='Examples Using the STOICH Module'

loopmax=1    check_con = 0

*****
* Keywords do not have spaces.
*
* Notes for stoich input:
* - It is best to use 1 for all flows. The composition then can be
*   thought of as a quantity. (There is no need for the composition to
*   add to one.)
* - Remember oils and solids are in kgs while gases (including oil gases)
*   are in mols.
* - Use negative composition values to indicate reactants.
* - It is necessary to set flows to some value (preferably one)
*   for all streams referenced even if they only contain computed
*   quantities.
*
*****
$MODULE = STOICH      desc= 'Coke Combustion'
               gs=gas1  ss=solid1
               s_base='Coke'

               h_bal=1 c_bal=1 s_bal=1 n_bal=1 o_bal=1
               gas=O2   gas=CO2   gas=H2O  gas=NO2   gas=SO2
               tmin = 273   tmax = 1273   dt=100

$INITGAS =GAS1   flow = 1.0 mol

$INITSOLID = SOLID1
               flow = 1.0 kg
               Coke=-1.0

*****
$MODULE = STOICH      desc= 'Kerogen-1 Pyrolysis (oil in gas)'
               gs=gas2  ss=solid2
```

```

s_base='KEROGEN-1'

h_bal=1 c_bal=1 s_bal=1 n_bal=1 o_bal=1

gas='H2' gas='C3H6'
solid='Char-S'
solid='Char-N'
solid='Char-O'

tmin = 273 tmax = 1273 dt=100

$INITGAS =GAS2 flow = 1.0 mol
ch4=1.3387 h2o=0.056366 c2h4=0.6905 h2s=0.01409
nh3=0.09864 oil-1=1.32812 oil-2=0.66582 oil-3=0.66582

$INITSOLID = SOLID2
flow = 1.0 kg
Kerogen-1=-1.0
Char-C=0.14442 Char-H=0.006036

```

OUTPUT FILE

Selected portions of the ASCII output file for this example are listed below.

```

%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%
Title : Examples Using the STOICH Module

Input file: stoich.inp

Time : 15:37:10
Date : 19-Nov-93

Model : osp
Version: 2.0
Machine: HP-9000

```

%%%%%%%%%%%%%



PROPERTY parameters

L

Species parameters :

L

Gas	C/mol	H/mol	O/mol	N/mol	S/mol	kg/mol	Dif-vol
1. N2	.00	.00	.00	2.00	.00	.0280	17.90
2. O2	.00	.00	2.00	.00	.00	.0320	16.60
3. H2	.00	2.00	.00	.00	.00	.0020	7.07
4. CO	1.00	.00	1.00	.00	.00	.0280	18.90
5. CO2	1.00	.00	2.00	.00	.00	.0440	26.90
6. H2O	.00	2.00	1.00	.00	.00	.0180	12.70
7. H2S	.00	2.00	.00	.00	1.00	.0340	21.00
8. SO2	.00	.00	2.00	.00	1.00	.0640	41.10
9. NH3	.00	3.00	.00	1.00	.00	.0170	14.90
10. NO2	.00	.00	2.00	1.00	.00	.0460	16.70
11. HCN	1.00	1.00	.00	1.00	.00	.0270	24.20
12. COS	1.00	.00	1.00	.00	1.00	.0600	39.00
13. CH4	1.00	4.00	.00	.00	.00	.0160	24.50
14. C2H4	2.00	4.00	.00	.00	.00	.0280	41.00
15. C2H6	2.00	6.00	.00	.00	.00	.0300	45.00
16. C3H6	3.00	6.00	.00	.00	.00	.0420	61.50
17. C3H8	3.00	8.00	.00	.00	.00	.0440	65.50
18. C5-pseudo	5.00	.00	.00	.00	.00	.0600	33.00
19. H12-pseudo	.00	12.00	.00	.00	.00	.0120	24.00
20. Oil-1	11.00	17.49	.22	.26	.03	.1578	228.00
21. Oil-2	24.00	38.16	.48	.57	.07	.3443	494.00
22. Oil-3	32.00	50.88	.64	.76	.10	.4590	664.00
23. Oil-4	20.00	31.20	.20	.38	.06	.2816	412.00
24. Oil-5	20.00	31.20	.20	.38	.06	.2816	412.00
25. Gas-A	.00	.00	.00	2.00	.00	.0280	17.90
26. Gas-B	.00	.00	.00	2.00	.00	.0280	17.90
27. Gas-C	.00	.00	.00	2.00	.00	.0280	17.90
28. Gas-D	.00	.00	.00	2.00	.00	.0280	17.90

L

Solid	W-frac C	W-frac H	W-frac O	W-frac N	W-frac S	kg/m**3	Inorg C
1. Kerogen-1	.8374	.1047	.0223	.0244	.0112	1050.0	.0000
2. Kerogen-2	1.0000	.0000	.0000	.0000	.0000	1000.0	.0000
3. Kerogen-3	1.0000	.0000	.0000	.0000	.0000	1000.0	.0000
4. Char-C	1.0000	.0000	.0000	.0000	.0000	1050.0	.0000
5. Char-H	.0000	1.0000	.0000	.0000	.0000	1050.0	.0000
6. Char-O	.0000	.0000	1.0000	.0000	.0000	1050.0	.0000
7. Char-N	.0000	.0000	.0000	1.0000	.0000	1050.0	.0000
8. Char-S	.0000	.0000	.0000	.0000	1.0000	1050.0	.0000
9. Inert	.0000	.0000	.0000	.0000	.0000	2650.0	.0000
10. Moisture	.0000	.1111	.9000	.0000	.0000	1000.0	.0000
11. Bound-water	.0000	.1111	.9000	.0000	.0000	1000.0	.0000
12. CaCO3	.1200	.0000	.4800	.0000	.0000	2710.0	.1200

13. CaO	.0000	.0000	.2857	.0000	.0000	3350.0	.0000
14. CaSO4	.0000	.0000	.4706	.0000	.2353	2960.0	.0000
15. MgCO3	.1424	.0000	.5694	.0000	.0000	2850.0	.1424
16. MgO	.0000	.0000	.3970	.0000	.0000	3580.0	.0000
17. MgSO4	.0000	.0000	.5320	.0000	.2660	2650.0	.0000
18. CaSiO3	.0000	.0000	.4138	.0000	.0000	2650.0	.0000
19. FeS2	.0000	.0000	.0000	.0000	.5342	4980.0	.0000
20. FeS	.0000	.0000	.0000	.0000	.3644	4830.0	.0000
21. Fe2O3	.0000	.0000	.3008	.0000	.0000	5280.0	.0000
22. SiO2	.0000	.0000	.5333	.0000	.0000	2650.0	.0000
23. N-inorganic	.0000	.0000	.0000	.0000	.0000	2650.0	.0000
24. Oil-1	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
25. Oil-2	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
26. Oil-3	.8367	.1108	.0223	.0233	.0069	1050.0	.0000
27. Oil-4	.8521	.1108	.0114	.0189	.0068	1050.0	.0000
28. Oil-5	.8521	.1108	.0114	.0189	.0068	1050.0	.0000
29. Coke	.9012	.0315	.0240	.0336	.0096	1050.0	.0000
30. Char	.8837	.0310	.0233	.0430	.0190	1050.0	.0000
31. Solid-A	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
32. Solid-B	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
33. Solid-C	.0000	.0000	.0000	.0000	.0000	2000.0	.0000
34. Solid-D	.0000	.0000	.0000	.0000	.0000	2000.0	.0000

|

Mod: 1) STOICH Coke Combustion Ver:1.01

Input values
Gases (stream 1)
Component mols
Solid (stream 1)
Component kgs
Coke -1.00000E+00

Balances used: Carbon Hydrogen Oxygen Nitrogen Sulfur

Gas(es) to balance:
2 - O2
5 - CO2
6 - H2O
10 - NO2
8 - SO2

Reaction Stoichiometry

(Note: Internal units are mols for gas & 'kgs for solids and liqs)

Component	Internal Units	kgs
O2(g)	-8.49250E+01	-2.71760E+00
CO2(g)	7.51000E+01	3.30440E+00
H2O(g)	1.57500E+01	2.83500E-01
SO2(g)	3.00000E-01	1.92000E-02
NO2(g)	2.40000E+00	1.10400E-01
Coke(s)	-1.00000E+00	-1.00000E+00

Heat of reaction

Temp (C)	HR
0.	-3.335E+07

100.	-3.343E+07
200.	-3.352E+07
300.	-3.364E+07
400.	-3.377E+07
500.	-3.392E+07
600.	-3.409E+07
700.	-3.427E+07
800.	-3.446E+07
900.	-3.466E+07
1000.	-3.486E+07

Mod: 2) STOICH Kerogen-1 Pyrolysis (oil in gas) Ver:1.01

Input values

Gases (stream 2)	
Component	mols
H2O	5.63660E-02
H2S	1.40900E-02
NH3	9.86400E-02
CH4	1.33870E+00
C2H4	6.90500E-01
Oil-1	1.32812E+00
Oil-2	6.65820E-01
Oil-3	6.65820E-01
Solid (stream 2)	
Component	kgs
Kerogen-1	-1.00000E+00
Char-C	1.44420E-01
Char-H	6.03600E-03

Balances used: Carbon Hydrogen Oxygen Nitrogen Sulfur

Gas(es) to balance:
3 - H2
16 - C3H6

Solid(s) to balance:
8 - Char-S
7 - Char-N
6 - Char-O

Reaction Stoichiometry

(Note: Internal units are mols for gas & 'kgs for solids and liqs)

Component	Internal Units	kgs
H2(g)	6.65075E-01	1.33015E-03
H2O(g)	5.63660E-02	1.01459E-03
H2S(g)	1.40900E-02	4.79060E-04
NH3(g)	9.86400E-02	1.67688E-03
CH4(g)	1.33870E+00	2.14192E-02
C2H4(g)	6.90500E-01	1.93340E-02
C3H6(g)	1.04446E+00	4.38675E-02
Oil-1(g)	1.32812E+00	2.09553E-01
Oil-2(g)	6.65820E-01	2.29209E-01
Oil-3(g)	6.65820E-01	3.05612E-01
Kerogen-1(s)	-1.00000E+00	-1.00000E+00
Char-C(s)	1.44420E-01	1.44420E-01
Char-H(s)	6.03600E-03	6.03600E-03
Char-O(s)	4.79167E-03	4.79167E-03
Char-N(s)	5.65489E-03	5.65489E-03

Char-S(s) 5.60111E-03 5.60111E-03

Heat of reaction

Temp (C)	HR
0.	2.132E+05
100.	1.882E+05
200.	1.636E+05
300.	1.444E+05
400.	1.354E+05
500.	1.414E+05
600.	1.675E+05
700.	2.184E+05
800.	2.991E+05
900.	4.144E+05
1000.	5.693E+05

Loop = 1 Run time (mins) = .03
STOICH STOICH
.00000 .00000

APPENDIX E

EXAMPLE: USING PROP_TAB MODULE

This is an example which uses a PROP_TAB module. The module is used to list properties of pure species and selected mixtures over a temperature range. The input file is listed in the "INPUT FILE" section and selected portions of the output file are listed in the "OUTPUT FILE" section.

In the \$GLOBAL section of the input file, LOOPMAX is set to one, since no iteration is required, and CHECK_CON is set to zero so that no stream connectivity check is done. A single PROP_TAB module is defined. Three mixture results are requested, one each solid, gas and liquid. The gas is essentially air, the solid is just the single solid species COKE and the liquid is a mixture of three oils. The stream initialization sections for these three mixtures only include composition information because mixture properties are only a function of temperature and composition. Results are presented on a per-unit-mass or -mole basis.

In the ASCII output file listing given below, computed results from the module are listed. Although perhaps not clear in this listing, the results of the PROP_TAB module calculations appear in a slightly different place in the output file than for most other modules. Because the module was not intended to simulate some physical operation, but rather to simply list properties, it operates differently than most other modules. All calculations are done during the initialization portion of the OSP simulation. The computed results are available and are output to the ASCII output file at the time the other modules are simply listing their input parameters. Note, as a consequence this tabular information are not recomputed as a result of changes in stream variables made by other modules.

The first section of the module's output list properties of pure species as a function of temperature. The enthalpies are relative to pure material at 25 °C. This is followed by a repeat of the module banner and compositional and property information on the mixtures of interest. Note, that only the composition information is meaningful in the gas/solid/liquid stream information area. The final tables give information about the mixture properties as a function of temperature.

INPUT FILE

Listing of full input file for this example is given below.

```
$GLOBAL      title='PROP_TAB Example'
loopmax=1    tol=1.0e-3  check_con = 0
*****
* Keywords do not have spaces.
```

```
*****
*****$MODULE = PROP_TAB      desc= 'Air, Coke & Oil Properties'
      gs=gas  ss=solid  ls=liquid
      tmin = 273   tmax = 1273   dt=100
$INITGAS=    GAS      flow=1.0  n2=0.79  o2=0.21 pres=1.5e5
$INITSOLID=  SOLID    flow=1.0  Coke=1.0
$INITLIQ=    LIQUID   flow=1.0  Oil-1=0.5  Oil-2=0.25  Oil-3=0.25
```

OUTPUT FILE

Selected portions of the ASCII output file for this example are listed below.

```
%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%
```

Title : PROP_TAB Example

Input file: prop_tab.inp

Time : 15:37:26
Date : 19-Nov-93

Model : osp
Version: 2.0
Machine: HP-9000

```
%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%
```



```
*****
Mod: 1) PROP_TAB          Air, Coke & Oil Properties      Ver:1.0
*****
```

Solid Species -----

Heat capacities (J/kg/K)

Temp (C)	Kerogen-1	Kerogen-2	Kerogen-3	Char-C	Char-H
.0	1.514E+03	1.500E+03	1.500E+03	6.572E+02	9.142E+03
100.0	1.929E+03	1.500E+03	1.500E+03	9.269E+02	1.085E+04
200.0	2.311E+03	1.500E+03	1.500E+03	1.160E+03	1.256E+04
300.0	2.659E+03	1.500E+03	1.500E+03	1.356E+03	1.426E+04
400.0	2.974E+03	1.500E+03	1.500E+03	1.515E+03	1.597E+04
500.0	3.256E+03	1.500E+03	1.500E+03	1.637E+03	1.768E+04
600.0	3.505E+03	1.500E+03	1.500E+03	1.722E+03	1.938E+04

700.0	3.720E+03	1.500E+03	1.500E+03	1.770E+03	2.109E+04
800.0	3.903E+03	1.500E+03	1.500E+03	1.782E+03	2.280E+04
900.0	4.052E+03	1.500E+03	1.500E+03	1.756E+03	2.451E+04
1000.0	4.168E+03	1.500E+03	1.500E+03	1.694E+03	2.621E+04
Temp (C)	Char-O	Char-N	Char-S	Inert	Moisture
.0	6.572E+02	6.572E+02	6.572E+02	7.067E+02	4.184E+03
100.0	9.269E+02	9.269E+02	9.269E+02	8.703E+02	4.184E+03
200.0	1.160E+03	1.160E+03	1.160E+03	9.763E+02	4.184E+03
300.0	1.356E+03	1.356E+03	1.356E+03	1.053E+03	4.184E+03
400.0	1.515E+03	1.515E+03	1.515E+03	1.109E+03	4.184E+03
500.0	1.637E+03	1.637E+03	1.637E+03	1.149E+03	4.184E+03
600.0	1.722E+03	1.722E+03	1.722E+03	1.173E+03	4.184E+03
700.0	1.770E+03	1.770E+03	1.770E+03	1.183E+03	4.184E+03
800.0	1.782E+03	1.782E+03	1.782E+03	1.179E+03	4.184E+03
900.0	1.756E+03	1.756E+03	1.756E+03	1.162E+03	4.184E+03
1000.0	1.694E+03	1.694E+03	1.694E+03	1.131E+03	4.184E+03
Temp (C)	Bound-water	CaCO3	CaO	CaSO4	MgCO3
.0	2.281E+03	7.322E+02	7.177E+02	7.119E+02	9.997E+02
100.0	2.501E+03	9.158E+02	8.162E+02	7.896E+02	1.260E+03
200.0	2.721E+03	1.011E+03	8.642E+02	8.639E+02	1.537E+03
300.0	2.941E+03	1.074E+03	8.935E+02	9.368E+02	1.833E+03
400.0	3.161E+03	1.122E+03	9.142E+02	1.009E+03	2.145E+03
500.0	3.381E+03	1.162E+03	9.303E+02	1.081E+03	2.476E+03
600.0	3.601E+03	1.198E+03	9.437E+02	1.153E+03	2.824E+03
700.0	3.821E+03	1.231E+03	9.553E+02	1.225E+03	3.190E+03
800.0	4.041E+03	1.263E+03	9.658E+02	1.297E+03	3.574E+03
900.0	4.261E+03	1.294E+03	9.753E+02	1.368E+03	3.975E+03
1000.0	4.481E+03	1.323E+03	9.842E+02	1.440E+03	4.394E+03
Temp (C)	MgO	MgSO4	CaSiO3	FeS2	FeS
.0	8.894E+02	1.073E+03	7.171E+02	4.930E+02	6.116E+02
100.0	1.033E+03	1.056E+03	8.450E+02	5.646E+02	6.230E+02
200.0	1.110E+03	1.078E+03	9.573E+02	5.947E+02	6.343E+02
300.0	1.162E+03	1.112E+03	1.054E+03	6.129E+02	6.456E+02
400.0	1.200E+03	1.152E+03	1.135E+03	6.284E+02	6.570E+02
500.0	1.229E+03	1.192E+03	1.201E+03	6.451E+02	6.683E+02
600.0	1.252E+03	1.233E+03	1.251E+03	6.646E+02	6.796E+02
700.0	1.269E+03	1.272E+03	1.286E+03	6.879E+02	6.909E+02
800.0	1.283E+03	1.310E+03	1.305E+03	7.155E+02	7.023E+02
900.0	1.292E+03	1.347E+03	1.309E+03	7.476E+02	7.136E+02
1000.0	1.297E+03	1.381E+03	1.297E+03	7.844E+02	7.249E+02
Temp (C)	Fe2O3	SiO2	N-inorganic	Oil-1	Oil-2
.0	6.632E+02	7.171E+02	6.572E+02	1.600E+03	1.600E+03
100.0	7.018E+02	8.450E+02	9.269E+02	1.600E+03	1.600E+03
200.0	7.897E+02	9.573E+02	1.160E+03	1.600E+03	1.600E+03
300.0	8.764E+02	1.054E+03	1.356E+03	1.600E+03	1.600E+03
400.0	9.456E+02	1.135E+03	1.515E+03	1.600E+03	1.600E+03
500.0	9.909E+02	1.201E+03	1.637E+03	1.600E+03	1.600E+03
600.0	1.009E+03	1.251E+03	1.722E+03	1.600E+03	1.600E+03
700.0	9.993E+02	1.286E+03	1.770E+03	1.600E+03	1.600E+03
800.0	9.601E+02	1.305E+03	1.782E+03	1.600E+03	1.600E+03
900.0	8.910E+02	1.309E+03	1.756E+03	1.600E+03	1.600E+03
1000.0	7.918E+02	1.297E+03	1.694E+03	1.600E+03	1.600E+03
Temp (C)	Oil-3	Oil-4	Oil-5	Coke	Char
.0	1.600E+03	1.600E+03	1.600E+03	1.514E+03	1.514E+03
100.0	1.600E+03	1.600E+03	1.600E+03	1.929E+03	1.929E+03
200.0	1.600E+03	1.600E+03	1.600E+03	2.311E+03	2.311E+03
300.0	1.600E+03	1.600E+03	1.600E+03	2.659E+03	2.659E+03
400.0	1.600E+03	1.600E+03	1.600E+03	2.974E+03	2.974E+03
500.0	1.600E+03	1.600E+03	1.600E+03	3.256E+03	3.256E+03

600.0	1.600E+03	1.600E+03	1.600E+03	3.505E+03	3.505E+03
700.0	1.600E+03	1.600E+03	1.600E+03	3.720E+03	3.720E+03
800.0	1.600E+03	1.600E+03	1.600E+03	3.903E+03	3.903E+03
900.0	1.600E+03	1.600E+03	1.600E+03	4.052E+03	4.052E+03
1000.0	1.600E+03	1.600E+03	1.600E+03	4.168E+03	4.168E+03
Temp (C)	Solid-A	Solid-B	Solid-C	Solid-D	
.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
100.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
200.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
300.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
400.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
500.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
600.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
700.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
800.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
900.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	
1000.0	1.000E+03	1.000E+03	1.000E+03	1.000E+03	

Enthalpy H-H298 (J/kg)

Temp (C)	Kerogen-1	Kerogen-2	Kerogen-3	Char-C	Char-H
.0	-3.929E+04	-3.772E+04	-3.772E+04	-1.731E+04	-2.348E+05
100.0	1.332E+05	1.123E+05	1.123E+05	6.220E+04	7.647E+05
200.0	3.454E+05	2.623E+05	2.623E+05	1.668E+05	1.935E+06
300.0	5.942E+05	4.123E+05	4.123E+05	2.929E+05	3.276E+06
400.0	8.761E+05	5.623E+05	5.623E+05	4.367E+05	4.788E+06
500.0	1.188E+06	7.123E+05	7.123E+05	5.946E+05	6.470E+06
600.0	1.526E+06	8.623E+05	8.623E+05	7.629E+05	8.323E+06
700.0	1.888E+06	1.012E+06	1.012E+06	9.378E+05	1.035E+07
800.0	2.269E+06	1.162E+06	1.162E+06	1.116E+06	1.254E+07
900.0	2.667E+06	1.312E+06	1.312E+06	1.293E+06	1.491E+07
1000.0	3.079E+06	1.462E+06	1.462E+06	1.466E+06	1.744E+07

Temp (C)	Char-O	Char-N	Char-S	Inert	Moisture
.0	-1.731E+04	-1.731E+04	-1.731E+04	-1.838E+04	-1.052E+05
100.0	6.220E+04	6.220E+04	6.220E+04	6.119E+04	3.132E+05
200.0	1.668E+05	1.668E+05	1.668E+05	1.538E+05	7.316E+05
300.0	2.929E+05	2.929E+05	2.929E+05	2.555E+05	1.150E+06
400.0	4.367E+05	4.367E+05	4.367E+05	3.637E+05	1.568E+06
500.0	5.946E+05	5.946E+05	5.946E+05	4.767E+05	1.987E+06
600.0	7.629E+05	7.629E+05	7.629E+05	5.929E+05	2.405E+06
700.0	9.378E+05	9.378E+05	9.378E+05	7.109E+05	2.824E+06
800.0	1.116E+06	1.116E+06	1.116E+06	8.291E+05	3.242E+06
900.0	1.293E+06	1.293E+06	1.293E+06	9.462E+05	3.660E+06
1000.0	1.466E+06	1.466E+06	1.466E+06	1.061E+06	4.079E+06

Temp (C)	Bound-water	CaCO3	CaO	CaSO4	MgCO3
.0	-5.799E+04	-1.921E+04	-1.848E+04	-1.814E+04	-2.588E+04
100.0	1.811E+05	6.441E+04	5.890E+04	5.699E+04	8.694E+04
200.0	4.421E+05	1.612E+05	1.432E+05	1.397E+05	2.266E+05
300.0	7.252E+05	2.656E+05	2.311E+05	2.297E+05	3.950E+05
400.0	1.030E+06	3.754E+05	3.216E+05	3.270E+05	5.937E+05
500.0	1.357E+06	4.897E+05	4.138E+05	4.315E+05	8.247E+05
600.0	1.706E+06	6.077E+05	5.075E+05	5.433E+05	1.090E+06
700.0	2.077E+06	7.292E+05	6.025E+05	6.622E+05	1.390E+06
800.0	2.470E+06	8.540E+05	6.986E+05	7.882E+05	1.728E+06
900.0	2.886E+06	9.818E+05	7.956E+05	9.215E+05	2.105E+06
1000.0	3.323E+06	1.113E+06	8.936E+05	1.062E+06	2.524E+06

Temp (C)	MgO	MgSO4	CaSiO3	FeS2	FeS
.0	-2.297E+04	-2.681E+04	-1.841E+04	-1.274E+04	-1.541E+04
100.0	7.401E+04	7.908E+04	5.983E+04	4.073E+04	4.631E+04

200.0	1.815E+05	1.856E+05	1.501E+05	9.886E+04	1.092E+05
300.0	2.952E+05	2.950E+05	2.508E+05	1.593E+05	1.732E+05
400.0	4.134E+05	4.082E+05	3.604E+05	2.214E+05	2.383E+05
500.0	5.348E+05	5.254E+05	4.773E+05	2.850E+05	3.046E+05
600.0	6.589E+05	6.467E+05	6.001E+05	3.505E+05	3.720E+05
700.0	7.850E+05	7.720E+05	7.271E+05	4.181E+05	4.405E+05
800.0	9.126E+05	9.011E+05	8.568E+05	4.882E+05	5.101E+05
900.0	1.041E+06	1.034E+06	9.877E+05	5.613E+05	5.809E+05
1000.0	1.171E+06	1.170E+06	1.118E+06	6.379E+05	6.529E+05
Temp (C)	Fe2O3	SiO2	N-inorganic	Oil-1	Oil-2
.0	-1.656E+04	-1.841E+04	-1.731E+04	-4.024E+04	-4.024E+04
100.0	5.085E+04	5.983E+04	6.220E+04	1.198E+05	1.198E+05
200.0	1.253E+05	1.501E+05	1.668E+05	2.798E+05	2.798E+05
300.0	2.087E+05	2.508E+05	2.929E+05	4.398E+05	4.398E+05
400.0	3.000E+05	3.604E+05	4.367E+05	5.998E+05	5.998E+05
500.0	3.970E+05	4.773E+05	5.946E+05	7.598E+05	7.598E+05
600.0	4.973E+05	6.001E+05	7.629E+05	9.198E+05	9.198E+05
700.0	5.980E+05	7.271E+05	9.378E+05	1.080E+06	1.080E+06
800.0	6.962E+05	8.568E+05	1.116E+06	1.240E+06	1.240E+06
900.0	7.890E+05	9.877E+05	1.293E+06	1.400E+06	1.400E+06
1000.0	8.734E+05	1.118E+06	1.466E+06	1.560E+06	1.560E+06
Temp (C)	Oil-3	Oil-4	Oil-5	Coke	Char
.0	-4.024E+04	-4.024E+04	-4.024E+04	-3.929E+04	-3.929E+04
100.0	1.198E+05	1.198E+05	1.198E+05	1.332E+05	1.332E+05
200.0	2.798E+05	2.798E+05	2.798E+05	3.454E+05	3.454E+05
300.0	4.398E+05	4.398E+05	4.398E+05	5.942E+05	5.942E+05
400.0	5.998E+05	5.998E+05	5.998E+05	8.761E+05	8.761E+05
500.0	7.598E+05	7.598E+05	7.598E+05	1.188E+06	1.188E+06
600.0	9.198E+05	9.198E+05	9.198E+05	1.526E+06	1.526E+06
700.0	1.080E+06	1.080E+06	1.080E+06	1.888E+06	1.888E+06
800.0	1.240E+06	1.240E+06	1.240E+06	2.269E+06	2.269E+06
900.0	1.400E+06	1.400E+06	1.400E+06	2.667E+06	2.667E+06
1000.0	1.560E+06	1.560E+06	1.560E+06	3.079E+06	3.079E+06
Temp (C)	Solid-A	Solid-B	Solid-C	Solid-D	
.0	-2.515E+04	-2.515E+04	-2.515E+04	-2.515E+04	
100.0	7.485E+04	7.485E+04	7.485E+04	7.485E+04	
200.0	1.749E+05	1.749E+05	1.749E+05	1.749E+05	
300.0	2.749E+05	2.749E+05	2.749E+05	2.749E+05	
400.0	3.749E+05	3.749E+05	3.749E+05	3.749E+05	
500.0	4.749E+05	4.749E+05	4.749E+05	4.749E+05	
600.0	5.749E+05	5.749E+05	5.749E+05	5.749E+05	
700.0	6.749E+05	6.749E+05	6.749E+05	6.749E+05	
800.0	7.749E+05	7.749E+05	7.749E+05	7.749E+05	
900.0	8.749E+05	8.749E+05	8.749E+05	8.749E+05	
1000.0	9.749E+05	9.749E+05	9.749E+05	9.749E+05	

Gas Species -----

Molecular weights (kg/mol):

N2	= .02800	O2	= .03200	H2	= .00200
CO	= .02800	CO2	= .04400	H2O	= .01800
H2S	= .03400	SO2	= .06400	NH3	= .01700
NO2	= .04600	HCN	= .02700	COS	= .06000
CH4	= .01600	C2H4	= .02800	C2H6	= .03000
C3H6	= .04200	C3H8	= .04400	C5-pseudo	= .06000
H12-pseudo	= .01200	Oil-1	= .15778	Oil-2	= .34425
Oil-3	= .45900	Oil-4	= .28164	Oil-5	= .28164
Gas-A	= .02800	Gas-B	= .02800	Gas-C	= .02800
Gas-D	= .02800				

Heat capacities (J/mol/K)

Temp (C)	N2	O2	H2	CO	CO2
.0	2.873E+01	2.898E+01	2.899E+01	2.870E+01	3.677E+01
100.0	2.925E+01	3.002E+01	2.904E+01	2.934E+01	4.016E+01
200.0	2.977E+01	3.100E+01	2.912E+01	2.997E+01	4.326E+01
300.0	3.030E+01	3.189E+01	2.925E+01	3.058E+01	4.606E+01
400.0	3.082E+01	3.271E+01	2.942E+01	3.118E+01	4.856E+01
500.0	3.134E+01	3.345E+01	2.963E+01	3.175E+01	5.076E+01
600.0	3.186E+01	3.411E+01	2.987E+01	3.232E+01	5.267E+01
700.0	3.238E+01	3.469E+01	3.016E+01	3.286E+01	5.429E+01
800.0	3.291E+01	3.520E+01	3.049E+01	3.339E+01	5.560E+01
900.0	3.343E+01	3.563E+01	3.086E+01	3.390E+01	5.662E+01
1000.0	3.395E+01	3.598E+01	3.127E+01	3.440E+01	5.734E+01
Temp (C)	H2O	H2S	SO2	NH3	NO2
.0	3.307E+01	3.347E+01	4.173E+01	3.506E+01	3.000E+01
100.0	3.411E+01	3.538E+01	4.666E+01	3.834E+01	3.000E+01
200.0	3.517E+01	3.723E+01	5.188E+01	4.149E+01	3.000E+01
300.0	3.626E+01	3.900E+01	5.740E+01	4.452E+01	3.000E+01
400.0	3.737E+01	4.071E+01	6.321E+01	4.742E+01	3.000E+01
500.0	3.850E+01	4.234E+01	6.931E+01	5.020E+01	3.000E+01
600.0	3.966E+01	4.390E+01	7.571E+01	5.285E+01	3.000E+01
700.0	4.084E+01	4.539E+01	8.240E+01	5.537E+01	3.000E+01
800.0	4.204E+01	4.680E+01	8.939E+01	5.777E+01	3.000E+01
900.0	4.327E+01	4.815E+01	9.667E+01	6.004E+01	3.000E+01
1000.0	4.452E+01	4.942E+01	1.042E+02	6.218E+01	3.000E+01
Temp (C)	HCN	COS	CH4	C2H4	C2H6
.0	3.000E+01	3.000E+01	3.342E+01	4.180E+01	4.958E+01
100.0	3.000E+01	3.000E+01	3.981E+01	5.141E+01	6.257E+01
200.0	3.000E+01	3.000E+01	4.584E+01	6.029E+01	7.464E+01
300.0	3.000E+01	3.000E+01	5.150E+01	6.844E+01	8.579E+01
400.0	3.000E+01	3.000E+01	5.681E+01	7.586E+01	9.601E+01
500.0	3.000E+01	3.000E+01	6.176E+01	8.255E+01	1.053E+02
600.0	3.000E+01	3.000E+01	6.635E+01	8.851E+01	1.137E+02
700.0	3.000E+01	3.000E+01	7.058E+01	9.374E+01	1.211E+02
800.0	3.000E+01	3.000E+01	7.445E+01	9.824E+01	1.276E+02
900.0	3.000E+01	3.000E+01	7.796E+01	1.020E+02	1.332E+02
1000.0	3.000E+01	3.000E+01	8.111E+01	1.051E+02	1.379E+02
Temp (C)	C3H6	C3H8	C5-pseudo	H12-pseudo	Oil-1
.0	6.087E+01	6.994E+01	5.733E+01	5.733E+01	2.826E+02
100.0	7.603E+01	8.913E+01	7.239E+01	7.239E+01	3.783E+02
200.0	9.005E+01	1.069E+02	8.628E+01	8.628E+01	4.791E+02
300.0	1.029E+02	1.231E+02	9.899E+01	9.899E+01	5.851E+02
400.0	1.146E+02	1.379E+02	1.105E+02	1.105E+02	6.962E+02
500.0	1.252E+02	1.512E+02	1.209E+02	1.209E+02	8.125E+02
600.0	1.346E+02	1.631E+02	1.301E+02	1.301E+02	9.340E+02
700.0	1.429E+02	1.735E+02	1.381E+02	1.381E+02	1.061E+03
800.0	1.500E+02	1.824E+02	1.450E+02	1.450E+02	1.192E+03
900.0	1.560E+02	1.898E+02	1.506E+02	1.506E+02	1.329E+03
1000.0	1.608E+02	1.958E+02	1.551E+02	1.551E+02	1.471E+03
Temp (C)	Oil-2	Oil-3	Oil-4	Oil-5	Gas-A
.0	6.123E+02	2.587E+02	6.000E+02	6.000E+02	3.000E+01
100.0	8.178E+02	3.276E+02	6.000E+02	6.000E+02	3.000E+01
200.0	1.034E+03	4.109E+02	6.000E+02	6.000E+02	3.000E+01
300.0	1.262E+03	5.085E+02	6.000E+02	6.000E+02	3.000E+01
400.0	1.500E+03	6.204E+02	6.000E+02	6.000E+02	3.000E+01
500.0	1.750E+03	7.468E+02	6.000E+02	6.000E+02	3.000E+01
600.0	2.010E+03	8.874E+02	6.000E+02	6.000E+02	3.000E+01
700.0	2.282E+03	1.042E+03	6.000E+02	6.000E+02	3.000E+01
800.0	2.565E+03	1.212E+03	6.000E+02	6.000E+02	3.000E+01

900.0	2.858E+03	1.396E+03	6.000E+02	6.000E+02	3.000E+01
1000.0	3.163E+03	1.594E+03	6.000E+02	6.000E+02	3.000E+01
Temp (C)	Gas-B	Gas-C	Gas-D		
.0	3.000E+01	3.000E+01	3.000E+01		
100.0	3.000E+01	3.000E+01	3.000E+01		
200.0	3.000E+01	3.000E+01	3.000E+01		
300.0	3.000E+01	3.000E+01	3.000E+01		
400.0	3.000E+01	3.000E+01	3.000E+01		
500.0	3.000E+01	3.000E+01	3.000E+01		
600.0	3.000E+01	3.000E+01	3.000E+01		
700.0	3.000E+01	3.000E+01	3.000E+01		
800.0	3.000E+01	3.000E+01	3.000E+01		
900.0	3.000E+01	3.000E+01	3.000E+01		
1000.0	3.000E+01	3.000E+01	3.000E+01		

Enthalpy H-H298 (J/mol)

Temp (C)	N2	O2	H2	CO	CO2
.0	-7.240E+02	-7.318E+02	-7.293E+02	-7.237E+02	-9.346E+02
100.0	2.175E+03	2.219E+03	2.172E+03	2.179E+03	2.914E+03
200.0	5.126E+03	5.270E+03	5.080E+03	5.145E+03	7.088E+03
300.0	8.129E+03	8.415E+03	7.998E+03	8.172E+03	1.156E+04
400.0	1.119E+04	1.165E+04	1.093E+04	1.126E+04	1.629E+04
500.0	1.429E+04	1.495E+04	1.388E+04	1.441E+04	2.126E+04
600.0	1.745E+04	1.833E+04	1.686E+04	1.761E+04	2.643E+04
700.0	2.067E+04	2.177E+04	1.986E+04	2.087E+04	3.178E+04
800.0	2.393E+04	2.527E+04	2.289E+04	2.418E+04	3.728E+04
900.0	2.725E+04	2.881E+04	2.596E+04	2.755E+04	4.289E+04
1000.0	3.062E+04	3.239E+04	2.906E+04	3.096E+04	4.859E+04
Temp (C)	H2O	H2S	SO2	NH3	NO2
.0	-8.348E+02	-8.472E+02	-1.064E+03	-8.911E+02	-7.545E+02
100.0	2.524E+03	2.596E+03	3.353E+03	2.780E+03	2.246E+03
200.0	5.988E+03	6.227E+03	8.278E+03	6.772E+03	5.246E+03
300.0	9.560E+03	1.004E+04	1.374E+04	1.107E+04	8.246E+03
400.0	1.324E+04	1.403E+04	1.977E+04	1.567E+04	1.125E+04
500.0	1.703E+04	1.818E+04	2.639E+04	2.055E+04	1.425E+04
600.0	2.094E+04	2.249E+04	3.364E+04	2.571E+04	1.725E+04
700.0	2.497E+04	2.696E+04	4.154E+04	3.112E+04	2.025E+04
800.0	2.911E+04	3.157E+04	5.013E+04	3.678E+04	2.325E+04
900.0	3.337E+04	3.631E+04	5.943E+04	4.267E+04	2.625E+04
1000.0	3.776E+04	4.119E+04	6.947E+04	4.878E+04	2.925E+04
Temp (C)	HCN	COS	CH4	C2H4	C2H6
.0	-7.545E+02	-7.545E+02	-8.590E+02	-1.079E+03	-1.285E+03
100.0	2.246E+03	2.246E+03	2.805E+03	3.587E+03	4.331E+03
200.0	5.246E+03	5.246E+03	7.091E+03	9.178E+03	1.120E+04
300.0	8.246E+03	8.246E+03	1.196E+04	1.562E+04	1.923E+04
400.0	1.125E+04	1.125E+04	1.738E+04	2.284E+04	2.833E+04
500.0	1.425E+04	1.425E+04	2.331E+04	3.077E+04	3.840E+04
600.0	1.725E+04	1.725E+04	2.972E+04	3.933E+04	4.936E+04
700.0	2.025E+04	2.025E+04	3.657E+04	4.845E+04	6.110E+04
800.0	2.325E+04	2.325E+04	4.382E+04	5.805E+04	7.355E+04
900.0	2.625E+04	2.625E+04	5.145E+04	6.807E+04	8.660E+04
1000.0	2.925E+04	2.925E+04	5.940E+04	7.843E+04	1.002E+05
Temp (C)	C3H6	C3H8	C5-pseudo	H12-pseudo	Oil-1
.0	-1.575E+03	-1.815E+03	-1.485E+03	-1.485E+03	-7.380E+03
100.0	5.280E+03	6.151E+03	5.010E+03	5.010E+03	2.562E+04
200.0	1.359E+04	1.596E+04	1.295E+04	1.295E+04	6.845E+04
300.0	2.325E+04	2.747E+04	2.223E+04	2.223E+04	1.216E+05
400.0	3.414E+04	4.054E+04	3.271E+04	3.271E+04	1.856E+05

500.0	4.614E+04	5.501E+04	4.429E+04	4.429E+04	2.610E+05
600.0	5.914E+04	7.073E+04	5.685E+04	5.685E+04	3.483E+05
700.0	7.303E+04	8.757E+04	7.027E+04	7.027E+04	4.480E+05
800.0	8.768E+04	1.054E+05	8.444E+04	8.444E+04	5.606E+05
900.0	1.030E+05	1.240E+05	9.923E+04	9.923E+04	6.867E+05
1000.0	1.188E+05	1.433E+05	1.145E+05	1.145E+05	8.267E+05
Temp (C)	Oil-2	Oil-3	Oil-4	Oil-5	Gas-A
.0	-1.598E+04	-6.700E+03	-1.509E+04	-1.509E+04	-7.545E+02
100.0	5.543E+04	2.250E+04	4.491E+04	4.491E+04	2.246E+03
200.0	1.479E+05	5.930E+04	1.049E+05	1.049E+05	5.246E+03
300.0	2.627E+05	1.051E+05	1.649E+05	1.649E+05	8.246E+03
400.0	4.007E+05	1.615E+05	2.249E+05	2.249E+05	1.125E+04
500.0	5.631E+05	2.297E+05	2.849E+05	2.849E+05	1.425E+04
600.0	7.510E+05	3.113E+05	3.449E+05	3.449E+05	1.725E+04
700.0	9.656E+05	4.077E+05	4.049E+05	4.049E+05	2.025E+04
800.0	1.208E+06	5.203E+05	4.649E+05	4.649E+05	2.325E+04
900.0	1.479E+06	6.505E+05	5.249E+05	5.249E+05	2.625E+04
1000.0	1.780E+06	7.999E+05	5.849E+05	5.849E+05	2.925E+04
Temp (C)	Gas-B	Gas-C	Gas-D		
.0	-7.545E+02	-7.545E+02	-7.545E+02		
100.0	2.246E+03	2.246E+03	2.246E+03		
200.0	5.246E+03	5.246E+03	5.246E+03		
300.0	8.246E+03	8.246E+03	8.246E+03		
400.0	1.125E+04	1.125E+04	1.125E+04		
500.0	1.425E+04	1.425E+04	1.425E+04		
600.0	1.725E+04	1.725E+04	1.725E+04		
700.0	2.025E+04	2.025E+04	2.025E+04		
800.0	2.325E+04	2.325E+04	2.325E+04		
900.0	2.625E+04	2.625E+04	2.625E+04		
1000.0	2.925E+04	2.925E+04	2.925E+04		

Viscosity (Pa-s)

Temp (C)	N2	O2	H2	CO	CO2
.0	1.730E-05	1.730E-05	8.300E-06	1.690E-05	1.360E-05
100.0	2.142E-05	2.142E-05	1.023E-05	2.083E-05	1.784E-05
200.0	2.521E-05	2.521E-05	1.200E-05	2.442E-05	2.194E-05
300.0	2.875E-05	2.875E-05	1.364E-05	2.777E-05	2.592E-05
400.0	3.210E-05	3.210E-05	1.519E-05	3.093E-05	2.982E-05
500.0	3.529E-05	3.529E-05	1.667E-05	3.394E-05	3.364E-05
600.0	3.836E-05	3.836E-05	1.809E-05	3.682E-05	3.739E-05
700.0	4.132E-05	4.132E-05	1.945E-05	3.960E-05	4.109E-05
800.0	4.418E-05	4.418E-05	2.077E-05	4.228E-05	4.474E-05
900.0	4.696E-05	4.696E-05	2.204E-05	4.488E-05	4.835E-05
1000.0	4.967E-05	4.967E-05	2.329E-05	4.741E-05	5.191E-05
Temp (C)	H2O	H2S	SO2	NH3	NO2
.0	8.800E-06	3.600E-05	3.600E-05	3.600E-05	3.600E-05
100.0	1.246E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
200.0	1.622E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
300.0	2.008E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
400.0	2.402E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
500.0	2.803E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
600.0	3.209E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
700.0	3.621E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
800.0	4.037E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
900.0	4.458E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
1000.0	4.883E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
Temp (C)	HCN	COS	CH4	C2H4	C2H6
.0	3.600E-05	3.600E-05	1.600E-05	3.600E-05	3.600E-05

100.0	3.600E-05	3.600E-05	2.028E-05	3.600E-05	3.600E-05
200.0	3.600E-05	3.600E-05	2.430E-05	3.600E-05	3.600E-05
300.0	3.600E-05	3.600E-05	2.811E-05	3.600E-05	3.600E-05
400.0	3.600E-05	3.600E-05	3.176E-05	3.600E-05	3.600E-05
500.0	3.600E-05	3.600E-05	3.529E-05	3.600E-05	3.600E-05
600.0	3.600E-05	3.600E-05	3.871E-05	3.600E-05	3.600E-05
700.0	3.600E-05	3.600E-05	4.203E-05	3.600E-05	3.600E-05
800.0	3.600E-05	3.600E-05	4.528E-05	3.600E-05	3.600E-05
900.0	3.600E-05	3.600E-05	4.845E-05	3.600E-05	3.600E-05
1000.0	3.600E-05	3.600E-05	5.156E-05	3.600E-05	3.600E-05
Temp (C)	C3H6	C3H8	C5-pseudo	H12-pseudo	Oil-1
.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
100.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
200.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
300.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
400.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
500.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
600.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
700.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
800.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
900.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
1000.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.600E-05
Temp (C)	Oil-2	Oil-3	Oil-4	Oil-5	Gas-A
.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	1.730E-05
100.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	2.142E-05
200.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	2.521E-05
300.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	2.875E-05
400.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.210E-05
500.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.529E-05
600.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	3.836E-05
700.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	4.132E-05
800.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	4.418E-05
900.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	4.696E-05
1000.0	3.600E-05	3.600E-05	3.600E-05	3.600E-05	4.967E-05
Temp (C)	Gas-B	Gas-C	Gas-D		
.0	1.730E-05	1.730E-05	1.730E-05		
100.0	2.142E-05	2.142E-05	2.142E-05		
200.0	2.521E-05	2.521E-05	2.521E-05		
300.0	2.875E-05	2.875E-05	2.875E-05		
400.0	3.210E-05	3.210E-05	3.210E-05		
500.0	3.529E-05	3.529E-05	3.529E-05		
600.0	3.836E-05	3.836E-05	3.836E-05		
700.0	4.132E-05	4.132E-05	4.132E-05		
800.0	4.418E-05	4.418E-05	4.418E-05		
900.0	4.696E-05	4.696E-05	4.696E-05		
1000.0	4.967E-05	4.967E-05	4.967E-05		

Liquid Species -----

Molecular weights (kg/mol):

Oil-1	= .15778	Oil-2	= .34425	Oil-3	= .45900
Oil-4	= .28164	Oil-5	= .28164	Water	= .01800
Liquid-A	= .01800	Liquid-B	= .01800		

Heat capacities (J/kg/K)

Temp (C)	Oil-1	Oil-2	Oil-3	Oil-4	Oil-5
.0	1.822E+03	1.812E+03	1.800E+03	6.748E+02	6.748E+02
100.0	2.438E+03	2.420E+03	2.402E+03	8.203E+02	8.203E+02
200.0	3.087E+03	3.061E+03	3.035E+03	9.734E+02	9.734E+02

300.0	3.769E+03	3.735E+03	3.700E+03	1.134E+03	1.134E+03
400.0	4.483E+03	4.441E+03	4.398E+03	1.303E+03	1.303E+03
500.0	5.230E+03	5.179E+03	5.126E+03	1.479E+03	1.479E+03
600.0	6.010E+03	5.951E+03	5.887E+03	1.663E+03	1.663E+03
700.0	6.823E+03	6.755E+03	6.680E+03	1.854E+03	1.854E+03
800.0	7.668E+03	7.591E+03	7.504E+03	2.053E+03	2.053E+03
900.0	8.547E+03	8.460E+03	8.360E+03	2.260E+03	2.260E+03
1000.0	9.458E+03	9.362E+03	9.248E+03	2.475E+03	2.475E+03

Temp (C)	Water	Liquid-A	Liquid-B
.0	4.184E+03	1.000E+03	1.000E+03
100.0	4.184E+03	1.000E+03	1.000E+03
200.0	4.184E+03	1.000E+03	1.000E+03
300.0	4.184E+03	1.000E+03	1.000E+03
400.0	4.184E+03	1.000E+03	1.000E+03
500.0	4.184E+03	1.000E+03	1.000E+03
600.0	4.184E+03	1.000E+03	1.000E+03
700.0	4.184E+03	1.000E+03	1.000E+03
800.0	4.184E+03	1.000E+03	1.000E+03
900.0	4.184E+03	1.000E+03	1.000E+03
1000.0	4.184E+03	1.000E+03	1.000E+03

Enthalpy H-H298 (J/kg)

Temp (C)	Oil-1	Oil-2	Oil-3	Oil-4	Oil-5
.0	-4.759E+04	-4.730E+04	-4.698E+04	-1.739E+04	-1.739E+04
100.0	1.652E+05	1.640E+05	1.628E+05	5.730E+04	5.730E+04
200.0	4.412E+05	4.378E+05	4.344E+05	1.469E+05	1.469E+05
300.0	7.837E+05	7.773E+05	7.709E+05	2.522E+05	2.522E+05
400.0	1.196E+06	1.186E+06	1.176E+06	3.740E+05	3.740E+05
500.0	1.681E+06	1.667E+06	1.651E+06	5.130E+05	5.130E+05
600.0	2.243E+06	2.223E+06	2.202E+06	6.701E+05	6.701E+05
700.0	2.885E+06	2.858E+06	2.830E+06	8.458E+05	8.458E+05
800.0	3.609E+06	3.575E+06	3.539E+06	1.041E+06	1.041E+06
900.0	4.419E+06	4.377E+06	4.332E+06	1.257E+06	1.257E+06
1000.0	5.319E+06	5.268E+06	5.212E+06	1.493E+06	1.493E+06

Temp (C)	Water	Liquid-A	Liquid-B
.0	-1.052E+05	-2.515E+04	-2.515E+04
100.0	3.132E+05	7.485E+04	7.485E+04
200.0	7.316E+05	1.749E+05	1.749E+05
300.0	1.150E+06	2.749E+05	2.749E+05
400.0	1.568E+06	3.749E+05	3.749E+05
500.0	1.987E+06	4.749E+05	4.749E+05
600.0	2.405E+06	5.749E+05	5.749E+05
700.0	2.824E+06	6.749E+05	6.749E+05
800.0	3.242E+06	7.749E+05	7.749E+05
900.0	3.660E+06	8.749E+05	8.749E+05
1000.0	4.079E+06	9.749E+05	9.749E+05

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*****
Module 1 : PROP_TAB          Air, Coke & Oil Properties
Tag :                      Group : 0           Version : 1.0
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Gas stream	GAS

Stream number	1 in
Flow (mol/s)	1.00E+00
Pressure (Pa)	1.50E+05
Temperature (C)	-273.15
Gas Composition (mol frac)	
N2	7.90E-01
O2	2.10E-01

H2	.00E+00
CO	.00E+00
CO2	.00E+00
H2O	.00E+00
H2S	.00E+00
SO2	.00E+00
NH3	.00E+00
NO2	.00E+00
HCN	.00E+00
COS	.00E+00
CH4	.00E+00
C2H4	.00E+00
C2H6	.00E+00
C3H6	.00E+00
C3H8	.00E+00
C5-pseudo	.00E+00
H12-pseudo	.00E+00
Oil-1	.00E+00
Oil-2	.00E+00
Oil-3	.00E+00
Oil-4	.00E+00
Oil-5	.00E+00
Gas-A	.00E+00
Gas-B	.00E+00
Gas-C	.00E+00
Gas-D	.00E+00

Solid stream	SOLID

Stream number	1 in
Flow (kg/min)	6.00E+01
Temp (C)	-273.15
Diameter (mm)	.000
Den (kg/m**3)	1050.0
Porosity	.00000
O Chr kg/m3	.00
O Ker kg/m3	.00
O FeS2 kg/m3	.00
Solid Comp. (wt. frac.)	
Kerogen-1	.00E+00
Kerogen-2	.00E+00
Kerogen-3	.00E+00
Char-C	.00E+00
Char-H	.00E+00
Char-O	.00E+00
Char-N	.00E+00
Char-S	.00E+00
Inert	.00E+00
Moisture	.00E+00
Bound-water	.00E+00
CaCO3	.00E+00
CaO	.00E+00
CaSO4	.00E+00
MgCO3	.00E+00
MgO	.00E+00
MgSO4	.00E+00
CaSiO3	.00E+00
FeS2	.00E+00
FeS	.00E+00
Fe2O3	.00E+00
SiO2	.00E+00
N-inorganic	.00E+00
Oil-1	.00E+00
Oil-2	.00E+00

Oil-3	.00E+00
Oil-4	.00E+00
Oil-5	.00E+00
Coke	1.00E+00
Char	.00E+00
Solid-A	.00E+00
Solid-B	.00E+00
Solid-C	.00E+00
Solid-D	.00E+00

Liquid stream	LIQUID
Stream number	1 in
Flow (kg/min)	6.00E+01
Temperature	-273.15
Liq Composition (wt frac)	
Oil-1	5.00E-01
Oil-2	2.50E-01
Oil-3	2.50E-01
Oil-4	.00E+00
Oil-5	.00E+00
Water	.00E+00
Liquid-A	.00E+00
Liquid-B	.00E+00

Solid Stream -----

Solid Stream 1 Enthalpy at 25 C = -8.8714E+01 J/kg

Temp (C)	Cp (J/kg/K)	Enth-Enth25C (J/kg)
.0	1.514E+03	-3.920E+04
100.0	1.929E+03	1.333E+05
200.0	2.311E+03	3.455E+05
300.0	2.659E+03	5.943E+05
400.0	2.974E+03	8.762E+05
500.0	3.256E+03	1.188E+06
600.0	3.505E+03	1.526E+06
700.0	3.720E+03	1.888E+06
800.0	3.903E+03	2.269E+06
900.0	4.052E+03	2.667E+06
1000.0	4.168E+03	3.079E+06

Gas Stream -----

Gas Stream 1 Enthalpy at 25 C = -4.1380E+00 J/mol

Temp (C)	Cp (J/mol/K)	Enth-Enth25C (J/mol)	Viscosity (Pa-s)
.0	2.878E+01	-7.215E+02	1.730E-05
100.0	2.941E+01	2.188E+03	2.142E-05
200.0	3.003E+01	5.161E+03	2.521E-05
300.0	3.063E+01	8.194E+03	2.875E-05
400.0	3.121E+01	1.129E+04	3.210E-05
500.0	3.178E+01	1.444E+04	3.529E-05
600.0	3.233E+01	1.764E+04	3.836E-05
700.0	3.287E+01	2.090E+04	4.132E-05
800.0	3.339E+01	2.422E+04	4.418E-05
900.0	3.389E+01	2.758E+04	4.696E-05
1000.0	3.438E+01	3.099E+04	4.967E-05

Liquid Stream -----

Liq Stream 1 Enthalpy at 25 C = -1.6576E+06 J/kg

Temp (C)	Cp (J/kg/K)	Enth-Enth25C (J/kg)
.0	1.814E+03	-4.722E+04
100.0	2.425E+03	1.644E+05
200.0	3.068E+03	4.388E+05
300.0	3.743E+03	7.791E+05
400.0	4.451E+03	1.188E+06
500.0	5.192E+03	1.670E+06
600.0	5.964E+03	2.228E+06
700.0	6.770E+03	2.864E+06
800.0	7.608E+03	3.583E+06
900.0	8.478E+03	4.387E+06
1000.0	9.381E+03	5.280E+06

Loop = 1 Run time (mins) = .04
PROP_TAB
.00000

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